

Supporting Material

Conversion of natural narciclasine to its C-1 and C-6 derivatives and their biological evaluation. Some unusual chemistry of narciclasine.

Juana Goulart Stollmaier^{1,*}, Jared Thomson¹, Mary Ann Endoma-Arias¹, Razvan Simionescu¹, Alexandra Vernaza², Nakya Mesa-Diaz², Mitchell Smith², Liqin Du², Alexander Kornienko^{2,*}, and Tomas Hudlicky¹

¹ Department of Chemistry, Brock University, 1812 Sir Isaac Brock Way, St. Catharines, ON L2S 3A1, Canada; jt15gq@brocku.ca (J.T.); maryann.arias@bpt.eurofinsca.com (M.A.E-A.); rsimionescu@brocku.ca (R.S.) thudlicky@brocku.ca (T.H.)

² Department of Chemistry and Biochemistry, Texas State University, San Marcos, TX 78666, USA; a_v651@txstate.edu (A.V.); nlm59@txstate.edu (N.M-D.); mts85@txstate.edu (M.S.); l_d141@txstate.edu (L.D.)

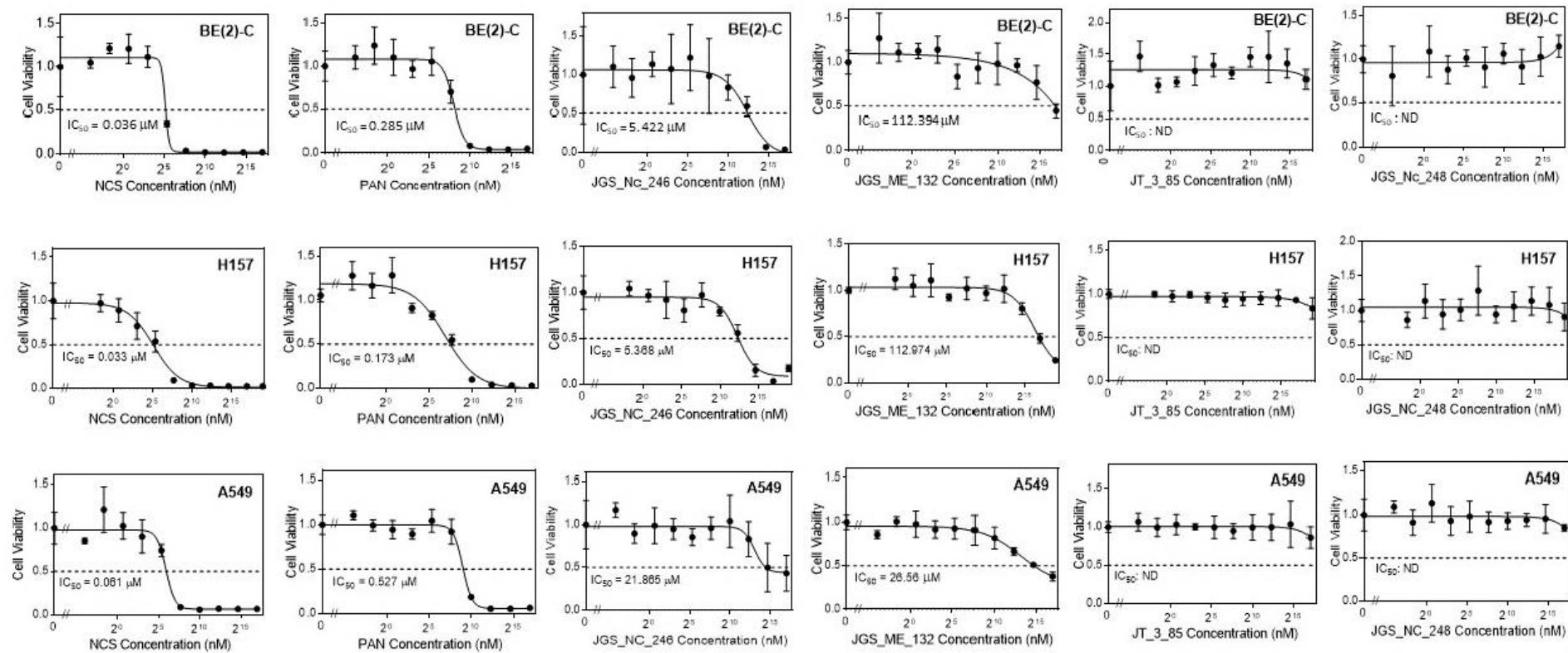
* Correspondence: juanagstollmaier@gmail.com (J.G.S); a_k76@txstate.edu (A.K.)

Table of Contents

Figure S1. Biological Activity.....	4
Selected Spectra	5
Figure S2. ^1H -NMR of 6	5
Figure S3. ^{13}C -NMR of 6	5
Figure S4. ^1H -NMR of 9	6
Figure S5. ^{13}C -NMR of 9	6
Figure S6. ^1H -NMR of 10	7
Figure S7. ^{13}C -NMR of 10	7
Figure S8. ^1H -NMR of 11	8
Figure S. ^{13}C -NMR of 11	8
Figure S10. ^1H -NMR of 12a	9
Figure S11. ^{13}C -NMR of 12a	9
Figure S12. ^1H -NMR of 12b	10
Figure S13. ^{13}C -NMR of 12b	10
Figure S14. ^1H -NMR of 14	11
Figure S15. ^{13}C -NMR of 14	11
Figure S16. ^1H -NMR of 15	12
Figure S17. ^{13}C -NMR of 15	12
Figure S18. ^1H -NMR of 16	13
Figure S19. ^{13}C -NMR of 16	14
Figure S20. ^1H -NMR of 17a	15
Figure S21. ^{13}C -NMR of 17a	15
Figure S22. ^1H -NMR of 24	16
Figure S23. ^{13}C -NMR of 24	16
Figure S24. ^1H - ^{15}N HSQC of 24	17
Figure S25. ^1H - ^{15}N HMBC of 24	17
Figure S26. ^1H -NMR of 25	18
Figure S27. ^{13}C -NMR of 25	18
Figure S28. ^{19}F -NMR of 25	19
Figure S29. ^1H -NMR of 26	20
Figure S30. ^{13}C -NMR of 26	20
Figure S31. ^1H - ^{15}N HMBC of 26	21

Figure S32. ^1H -NMR of 27	22
Figure S33. ^{13}C -NMR of 27	22
Figure S34. ^1H -NMR of 28	23
Figure S35. ^{13}C -NMR of 28	23
Figure S36. ^1H -NMR of 29	24
Figure S37. ^{13}C -NMR of 29	24
Figure S38. ^1H -NMR of 30	25
Figure S39. ^{13}C -NMR of 30	25
Figure S40. ^1H -NMR of 31	26
Figure S41. ^{13}C -NMR of 31	26
Figure S42. ^1H -NMR of 33	27
Figure S43. ^{13}C -NMR of 33	27

Figure S1. Biological Activity



Suppl. Figure S1. Dose-dependent cytotoxicity of compounds in cancer cell lines. Cells were treated with a serial of dilutions of each compound in three replicates in 96-well plates for 4 days, and cell viability was measured using MTT assay. Shown in each figure is dose-dependent response of the indicated cells to the indicated compound, with the dotted line signifying the IC_{50} . ND, not determined ($>500 \mu M$). NCS = 1, PAN = 2, JGS_Nc_246 = 29, JGS_ME_132 = 30, JT_3_85 = 31, JGS_Nc_248 = 33.

Selected Spectra

Figure S2. ^1H -NMR of **6**

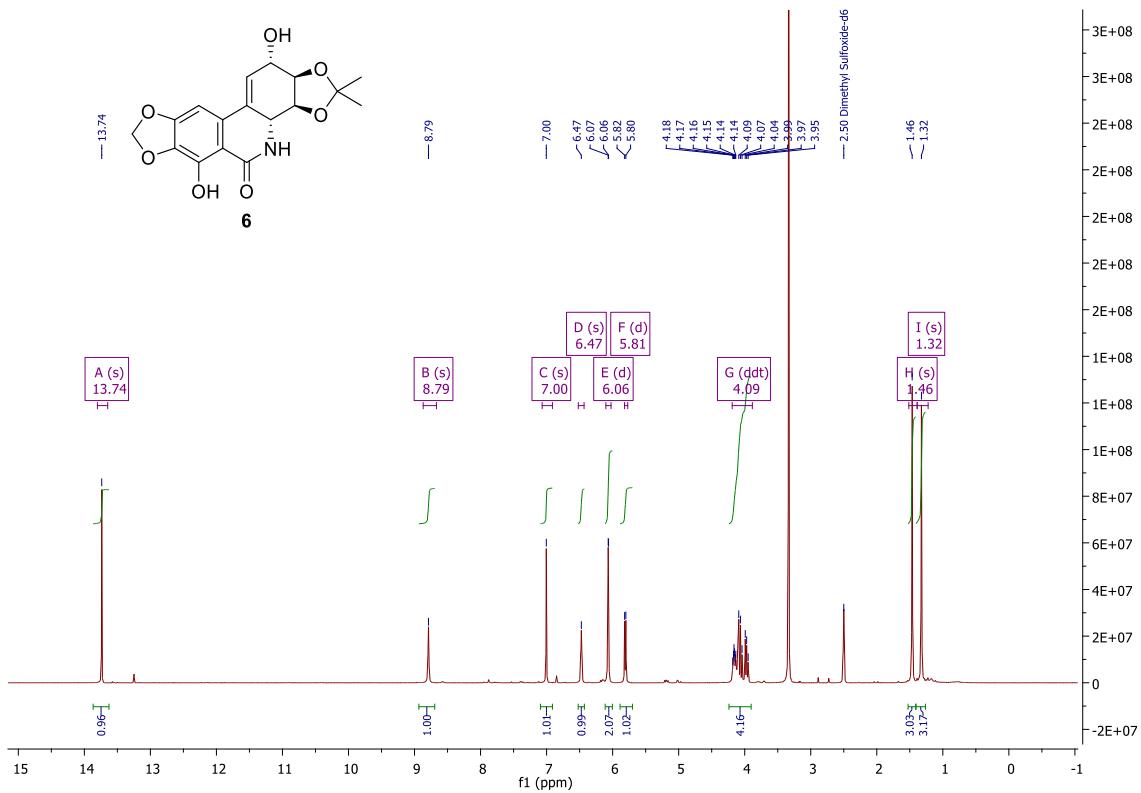


Figure S3. ^{13}C -NMR of **6**

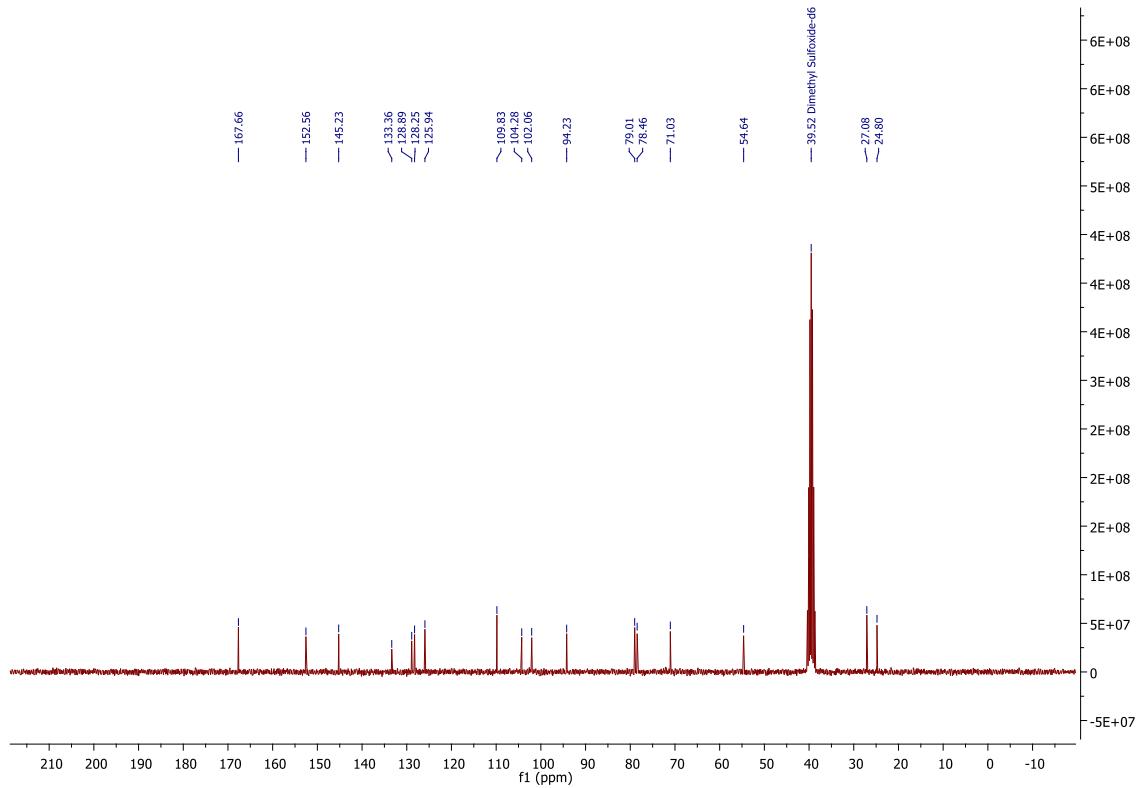


Figure S4. ^1H -NMR of **9**

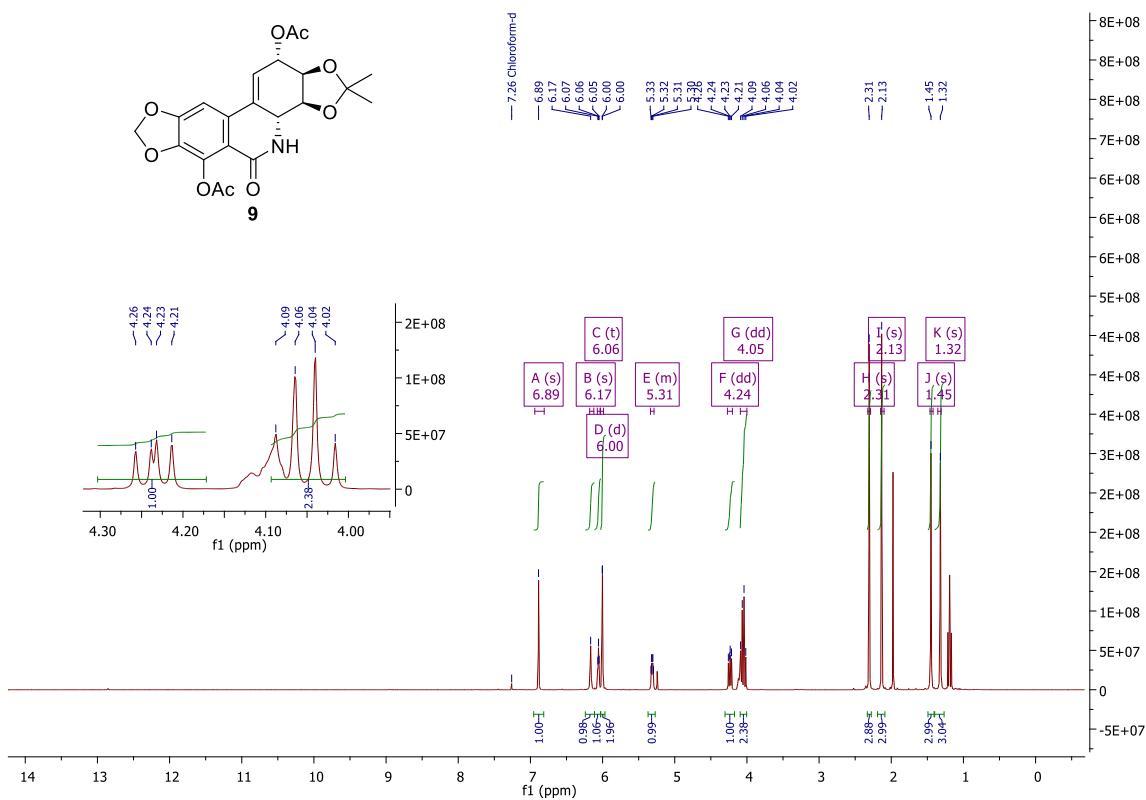


Figure S5. ^{13}C -NMR of **9**

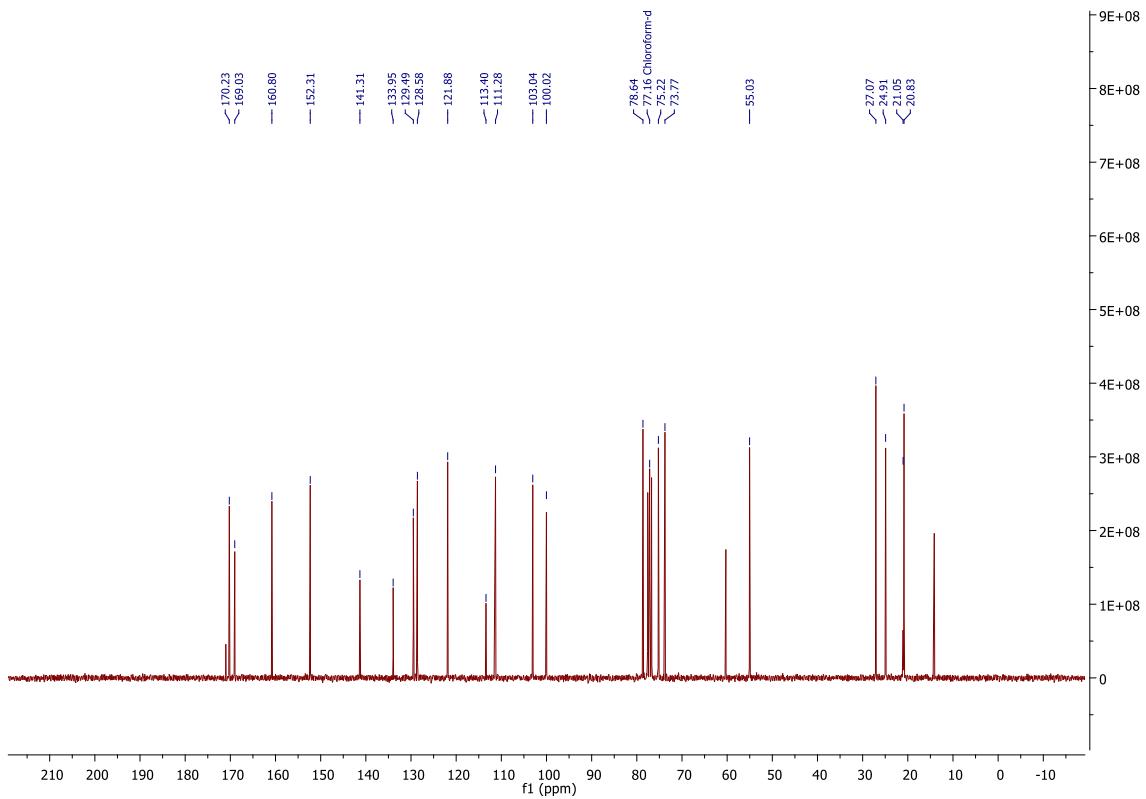


Figure S6. ^1H -NMR of **10**

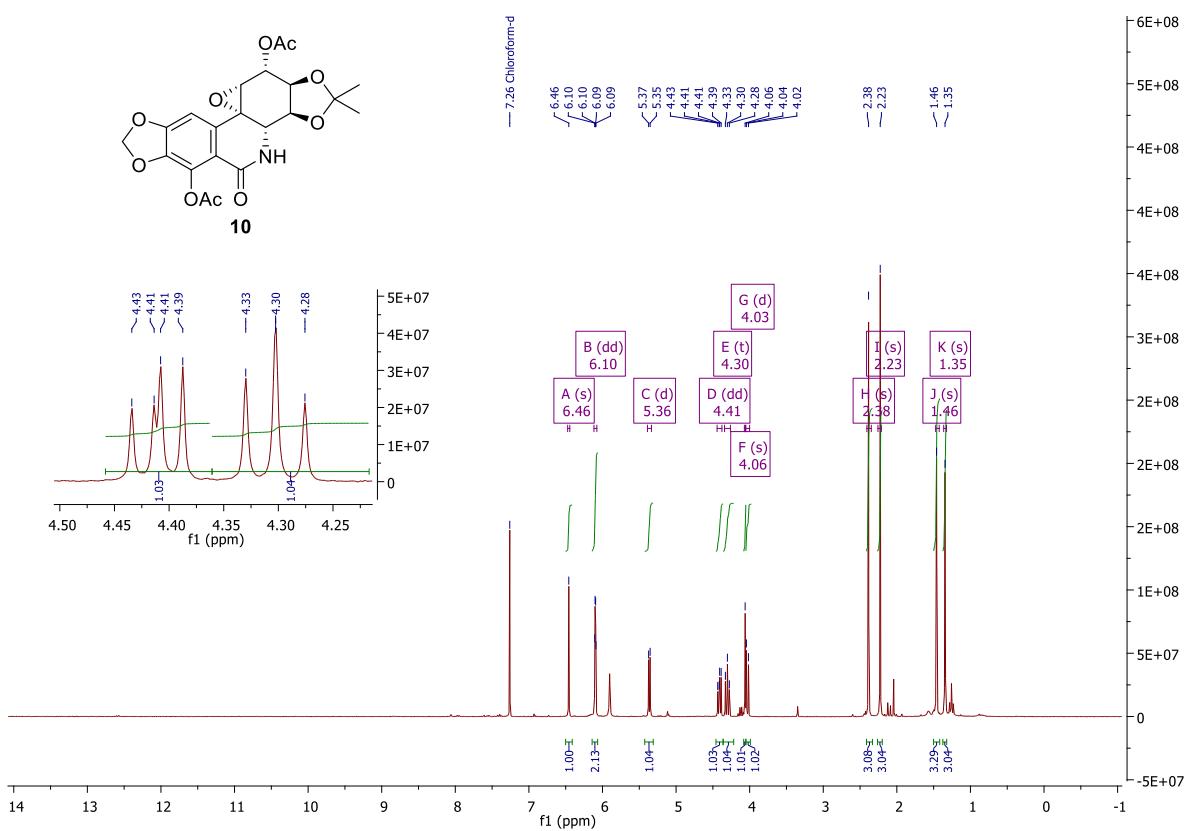


Figure S7. ^{13}C -NMR of **10**

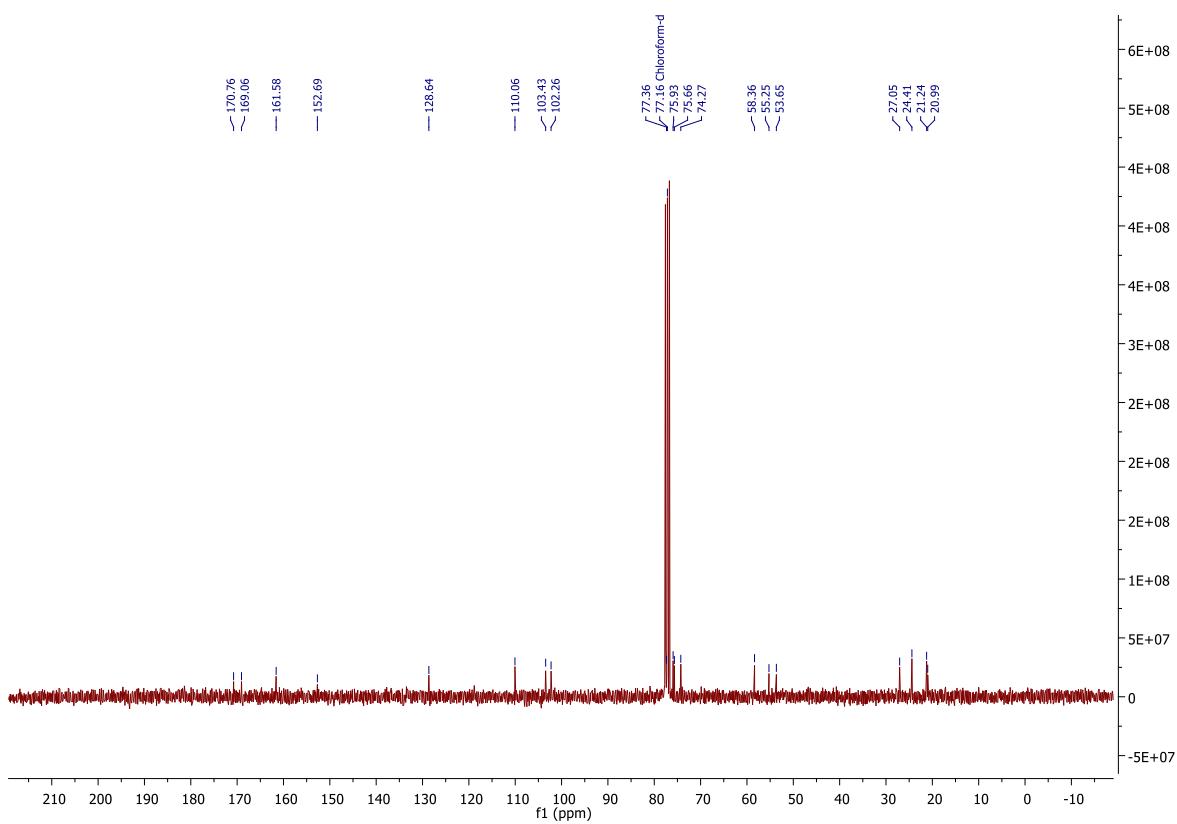


Figure S8. ^1H -NMR of **11**

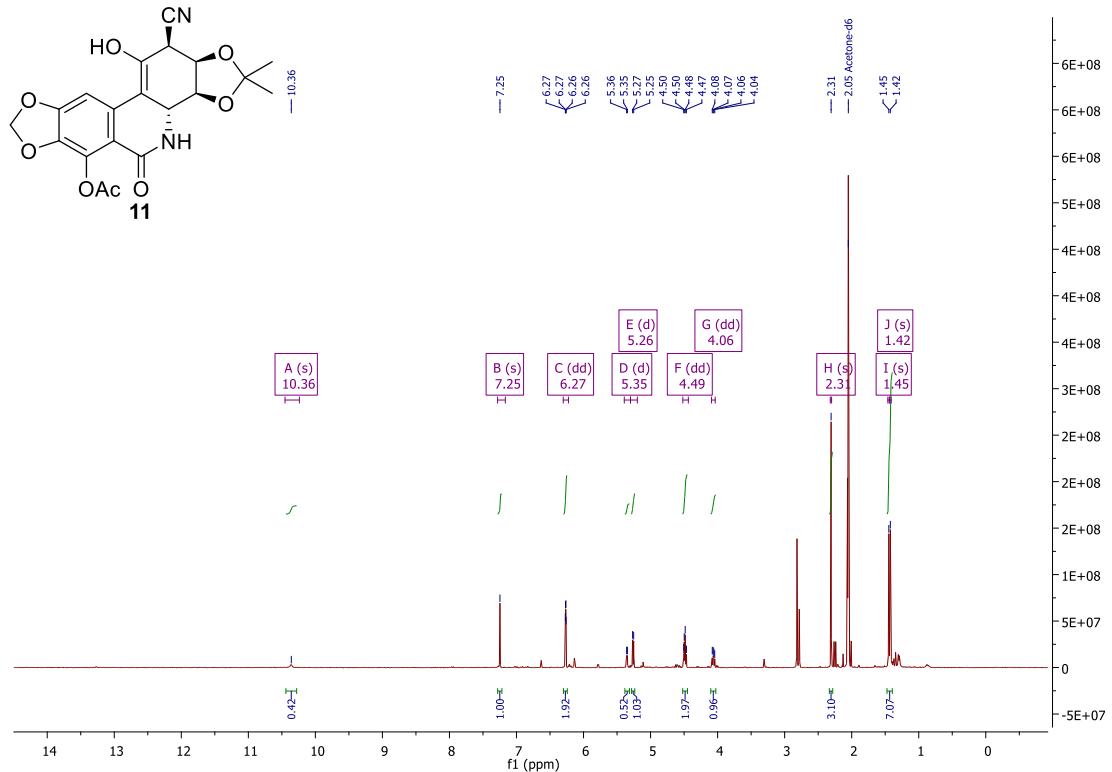


Figure S9. ^{13}C -NMR of **11**

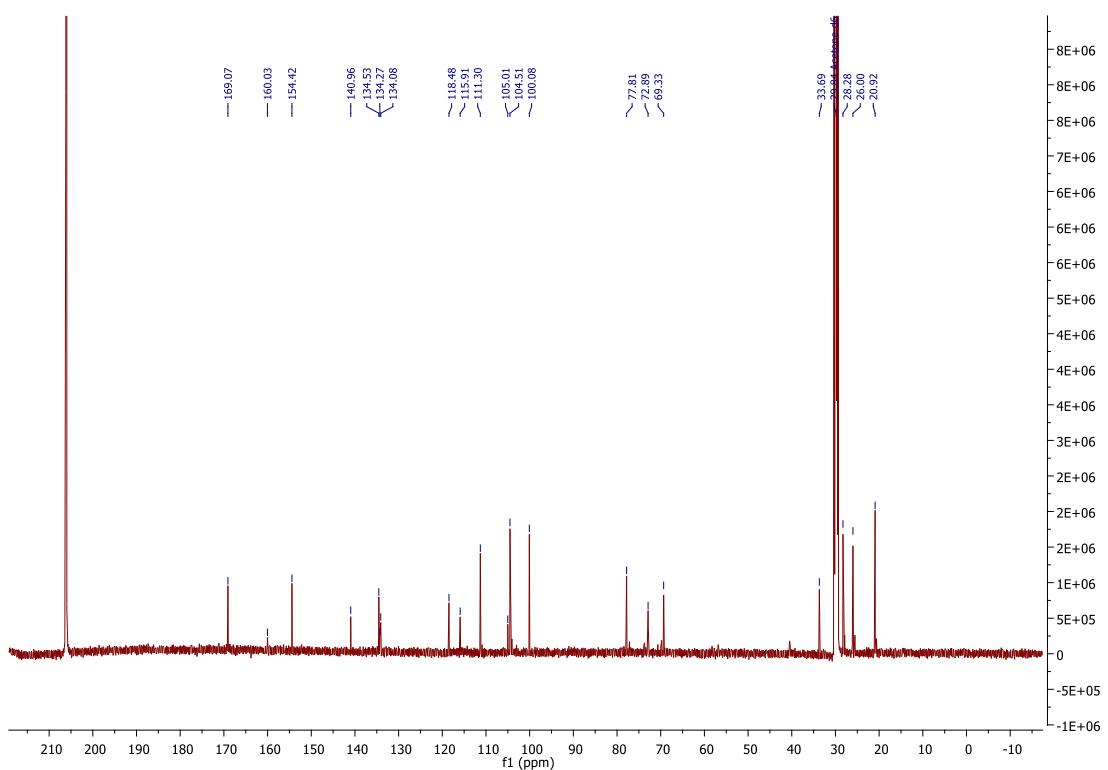


Figure S10. ^1H -NMR of **12a**

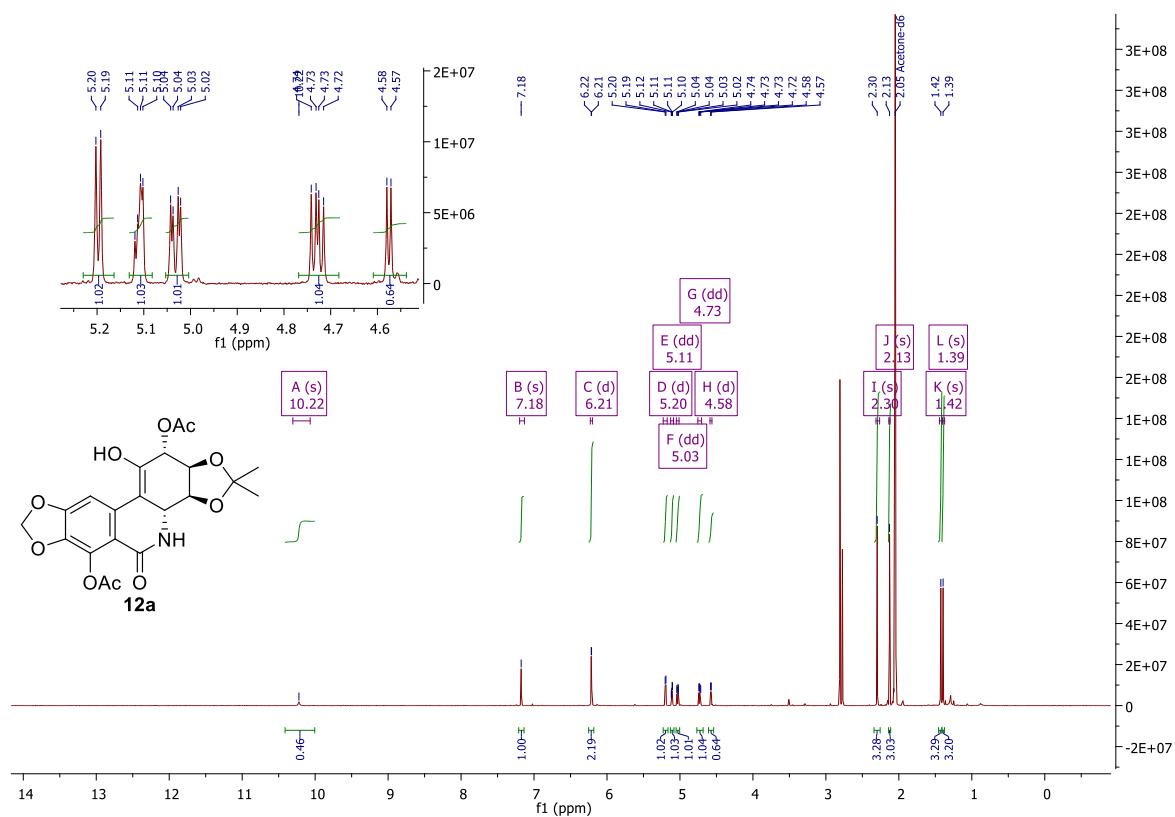


Figure S11. ^{13}C -NMR of **12a**

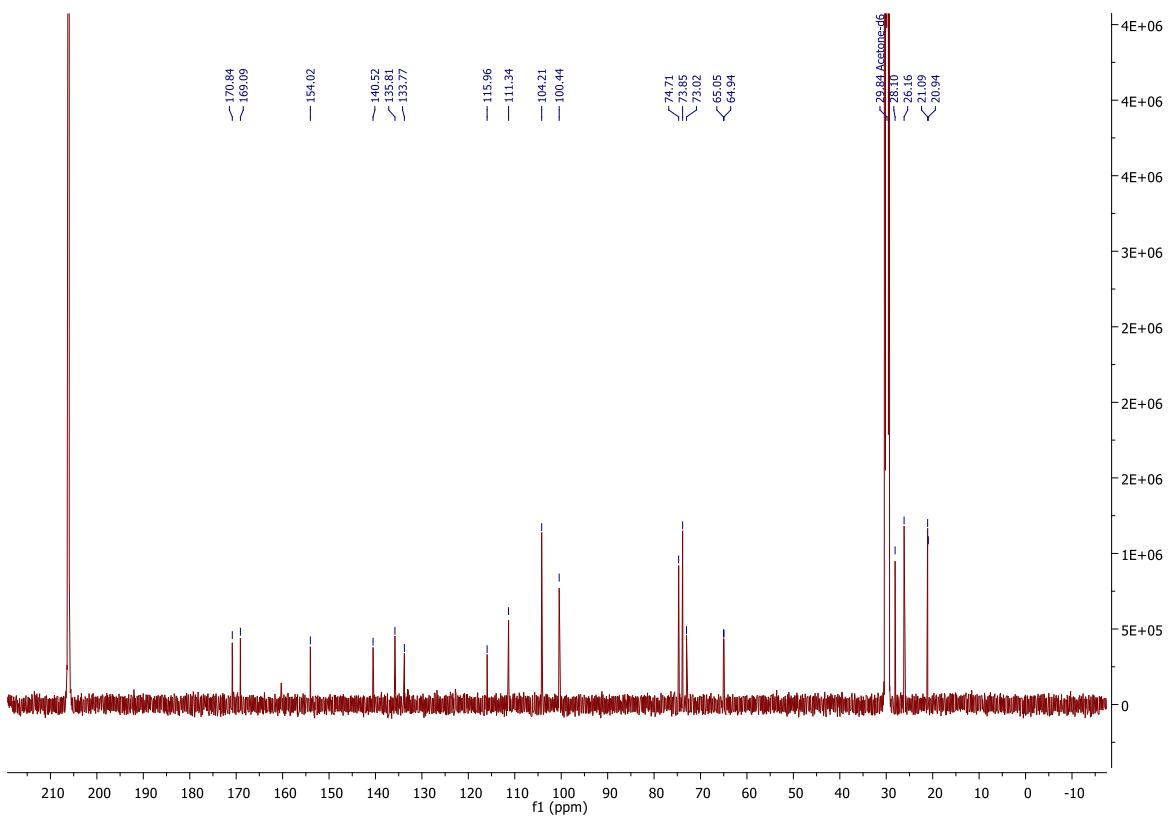


Figure S12. ^1H -NMR of **12b**

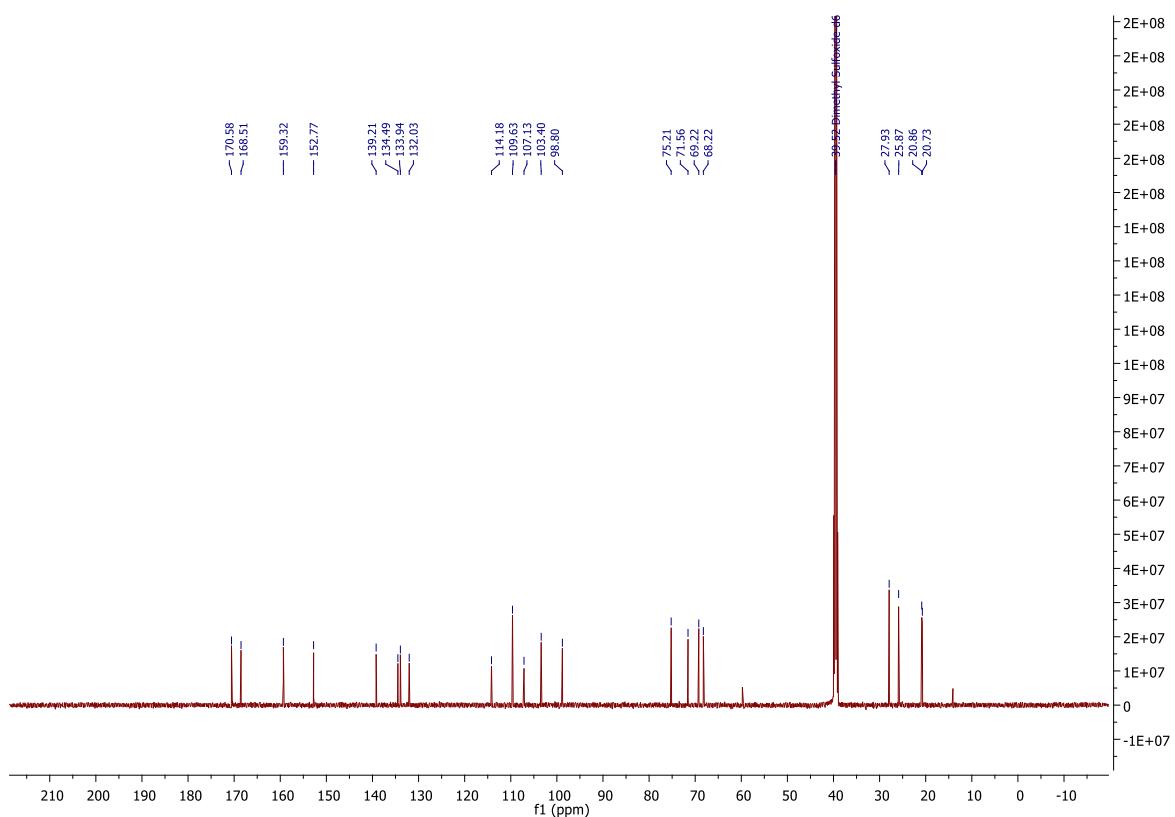
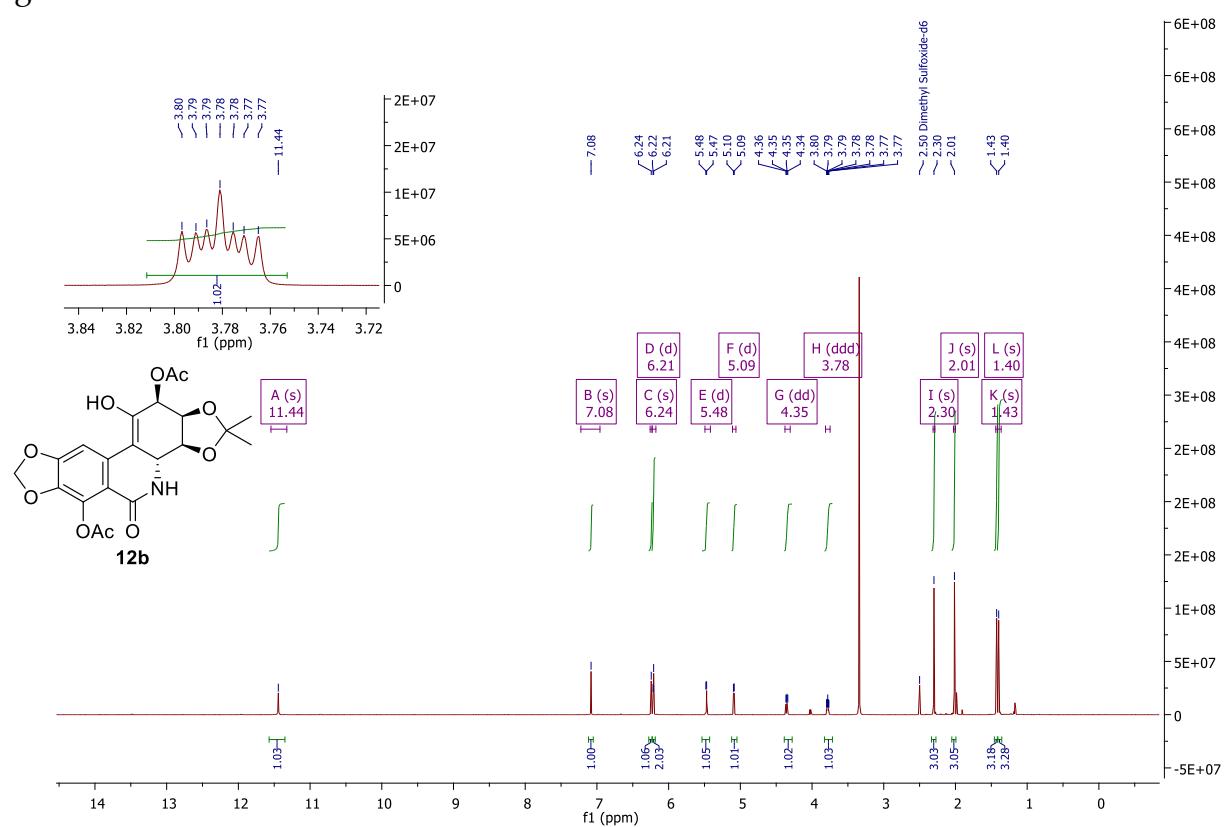


Figure S14. ^1H -NMR of **14**

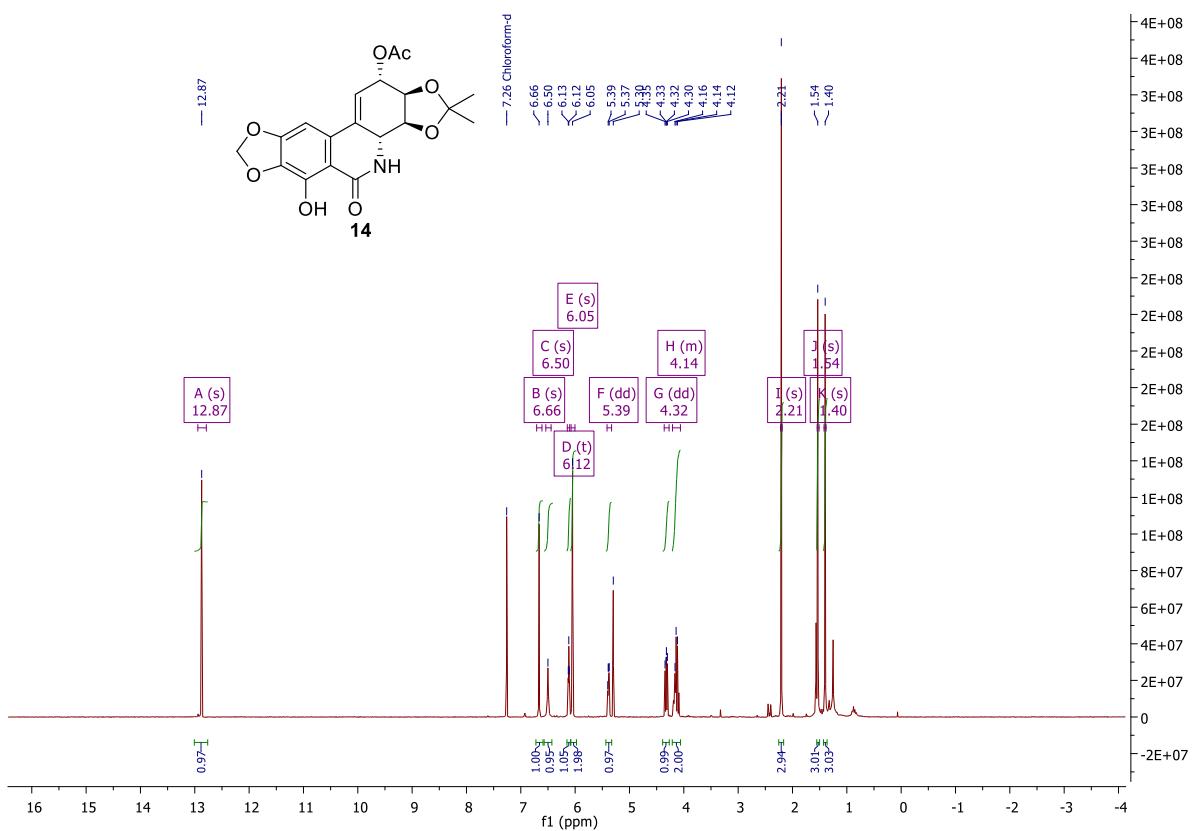


Figure S15. ^{13}C -NMR of **14**

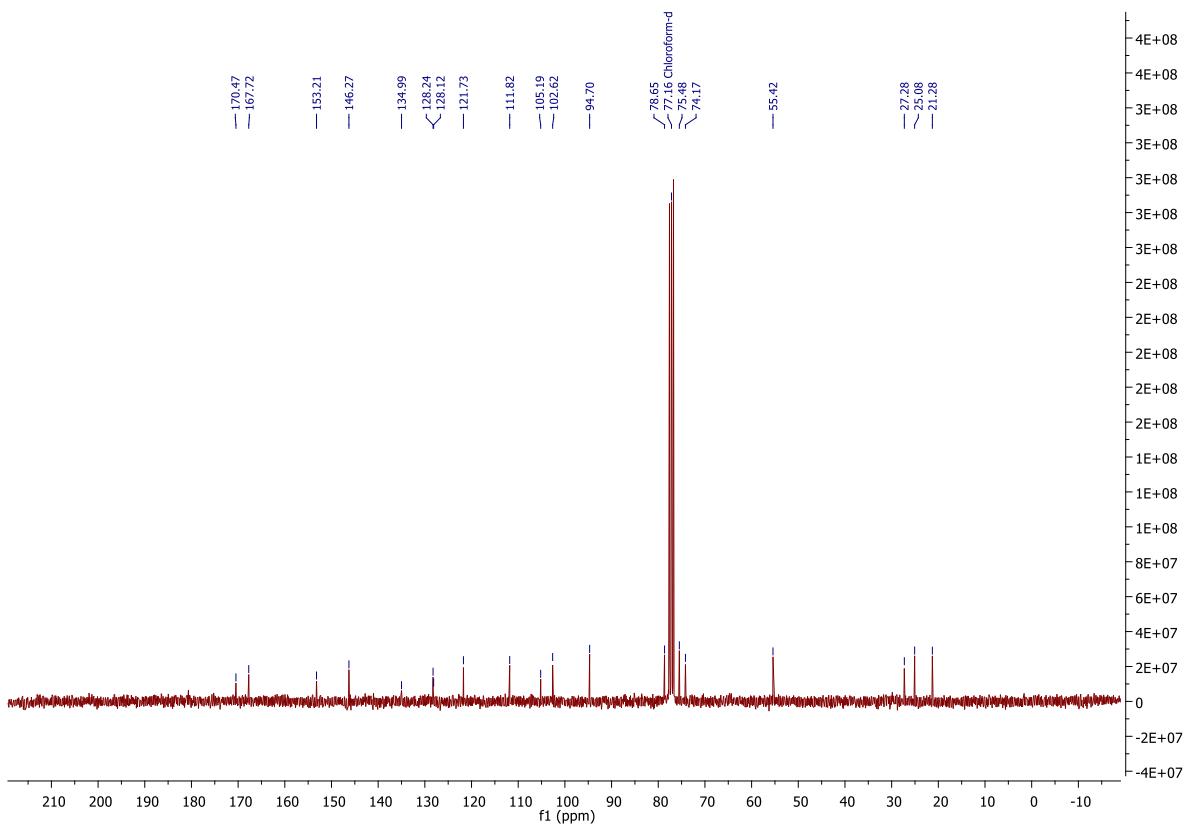


Figure S16. ^1H -NMR of **15**

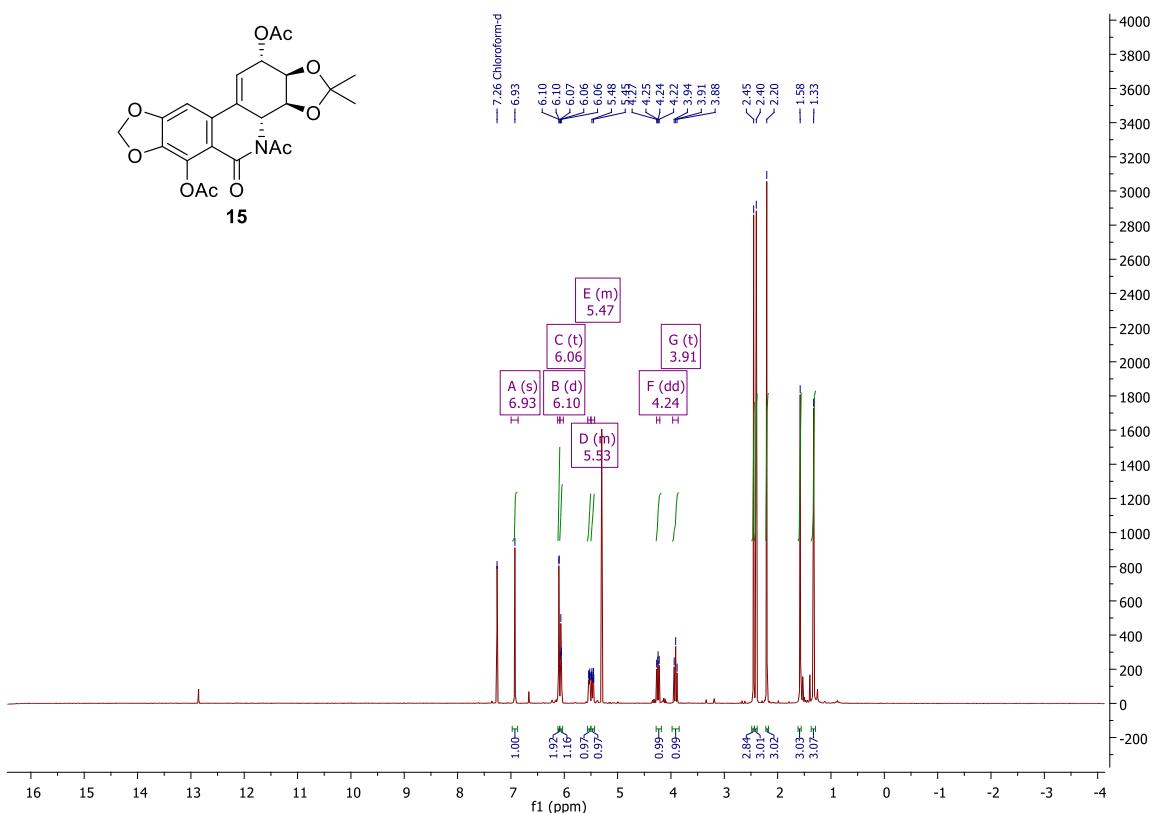


Figure S17. ^{13}C -NMR of **15**

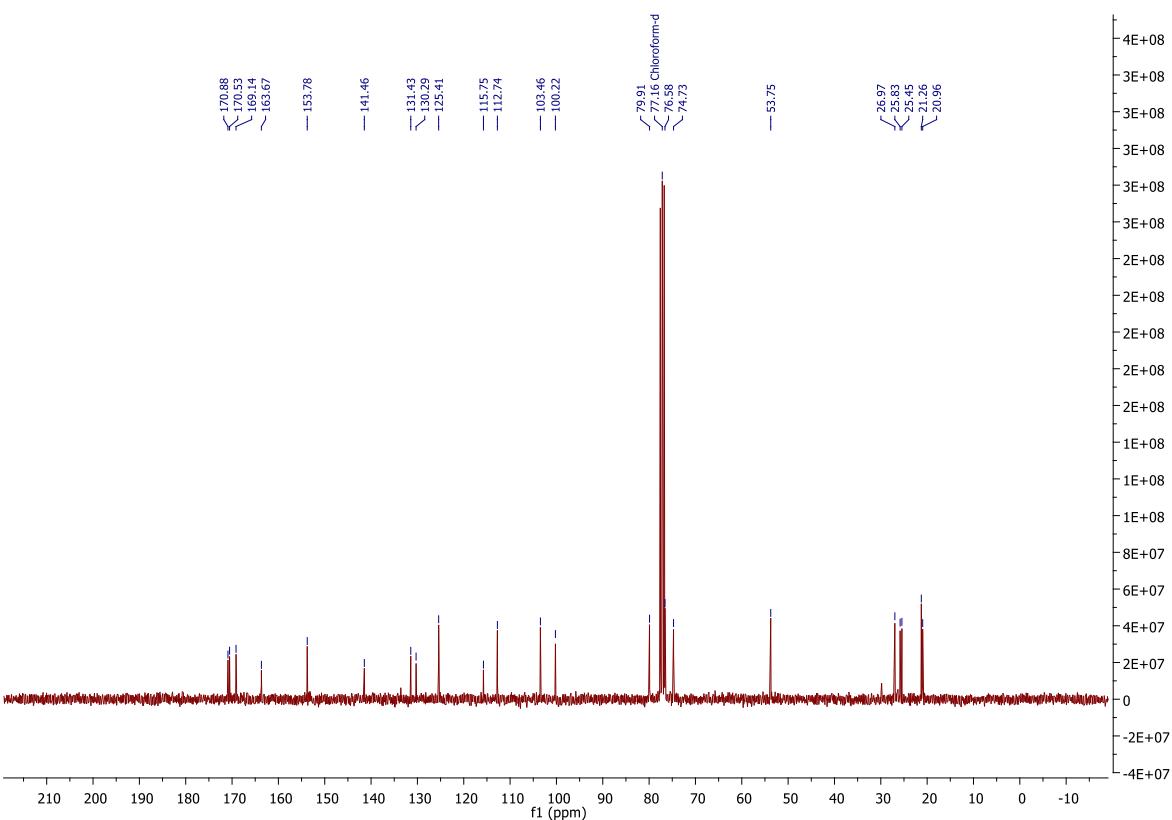


Figure S18. ^1H -NMR of **16**

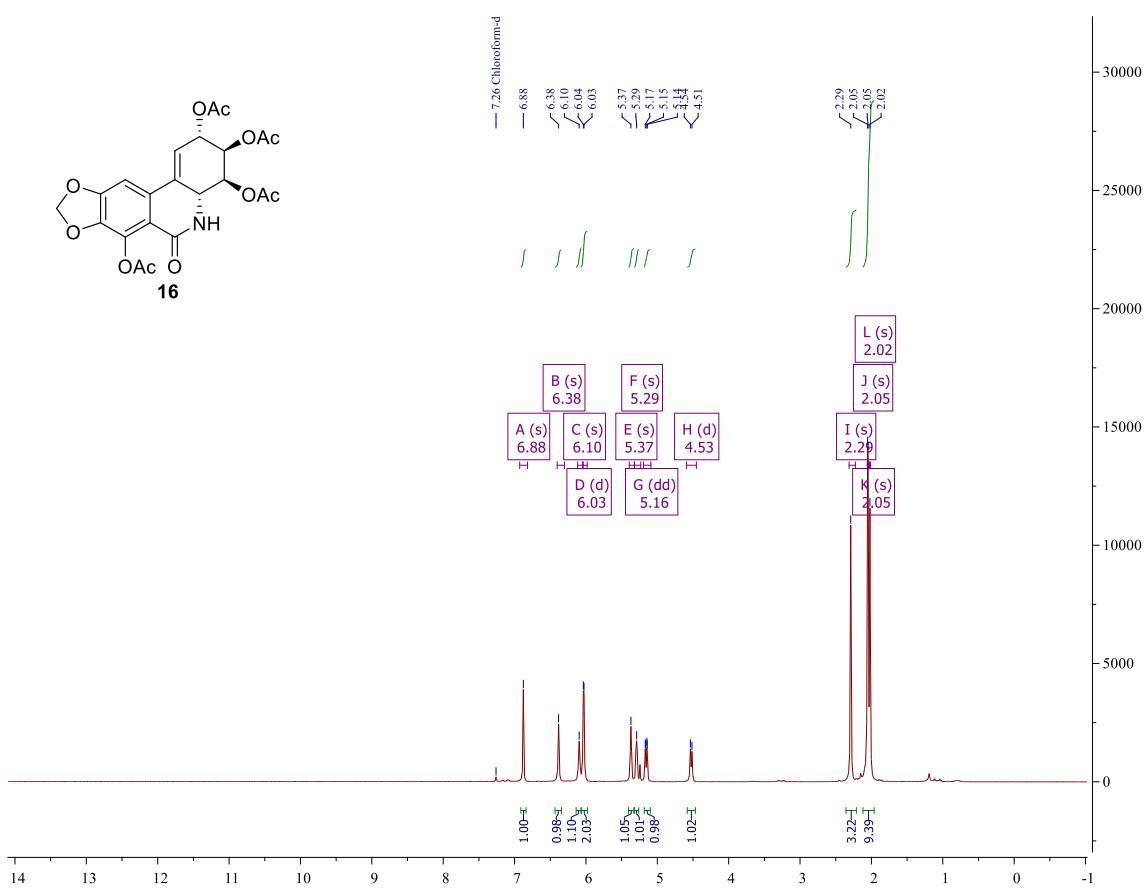


Figure S19. ^{13}C -NMR of **16**

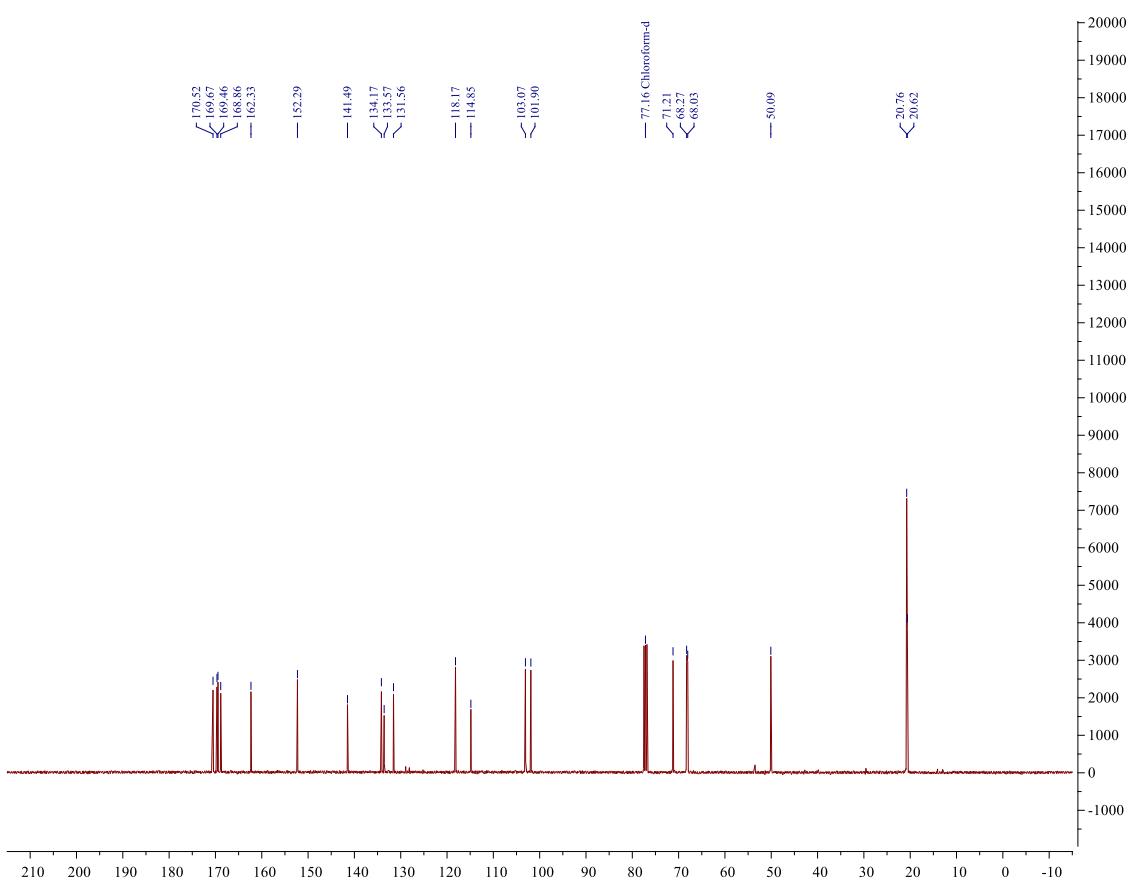


Figure S20. ^1H -NMR of **17a**

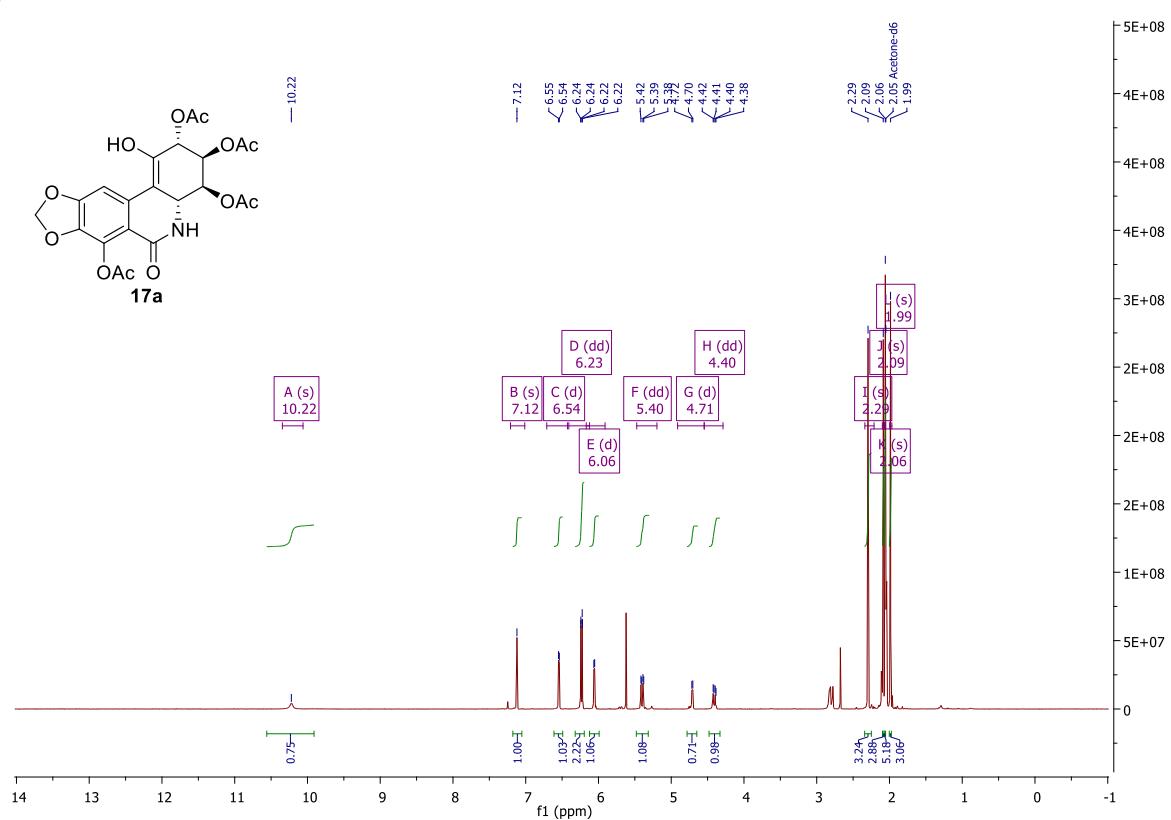


Figure S21. ^{13}C -NMR of **17a**

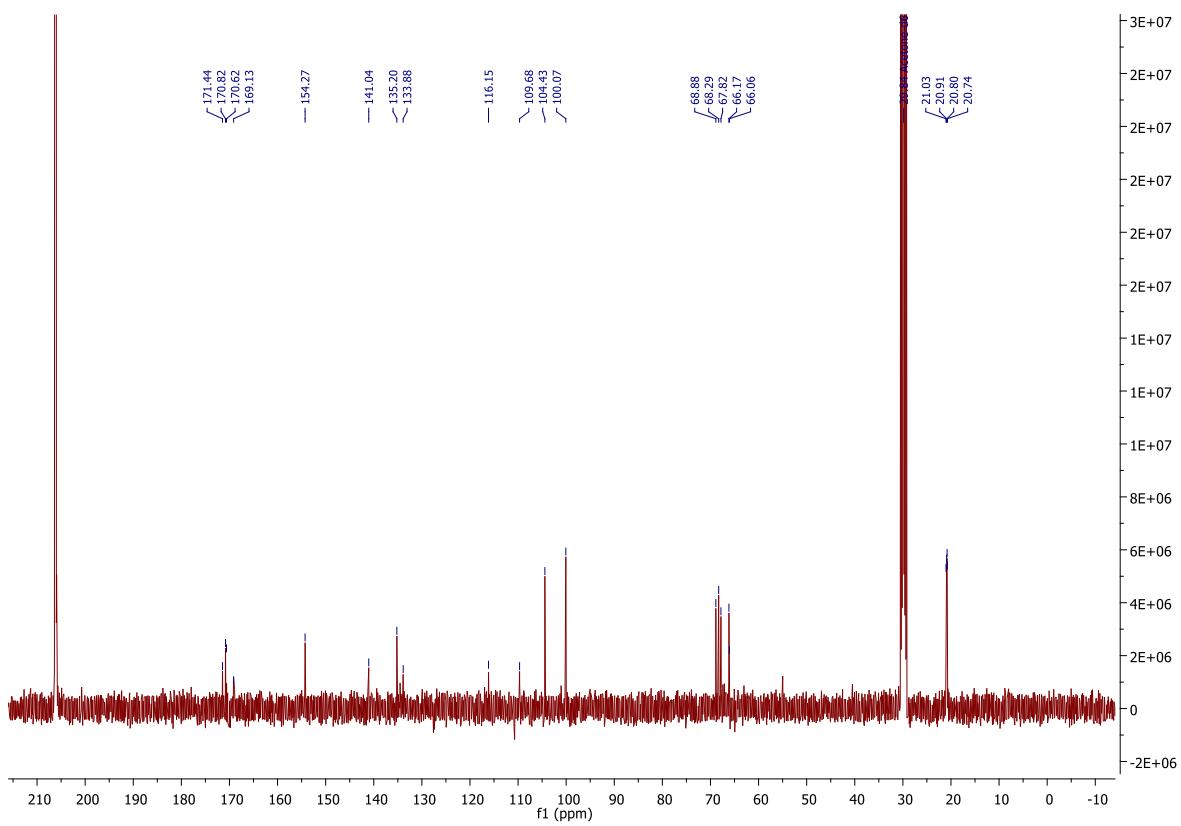


Figure S22. ^1H -NMR of **24**

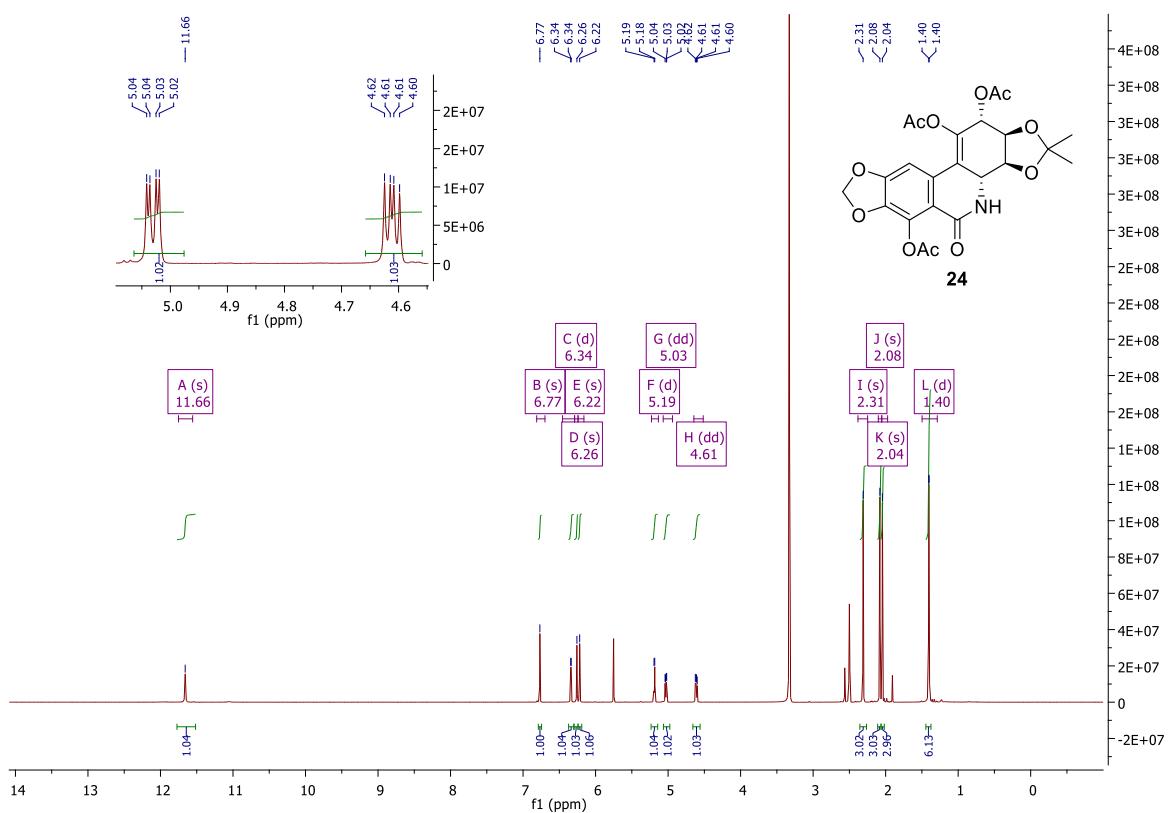


Figure S23. ^{13}C -NMR of **24**

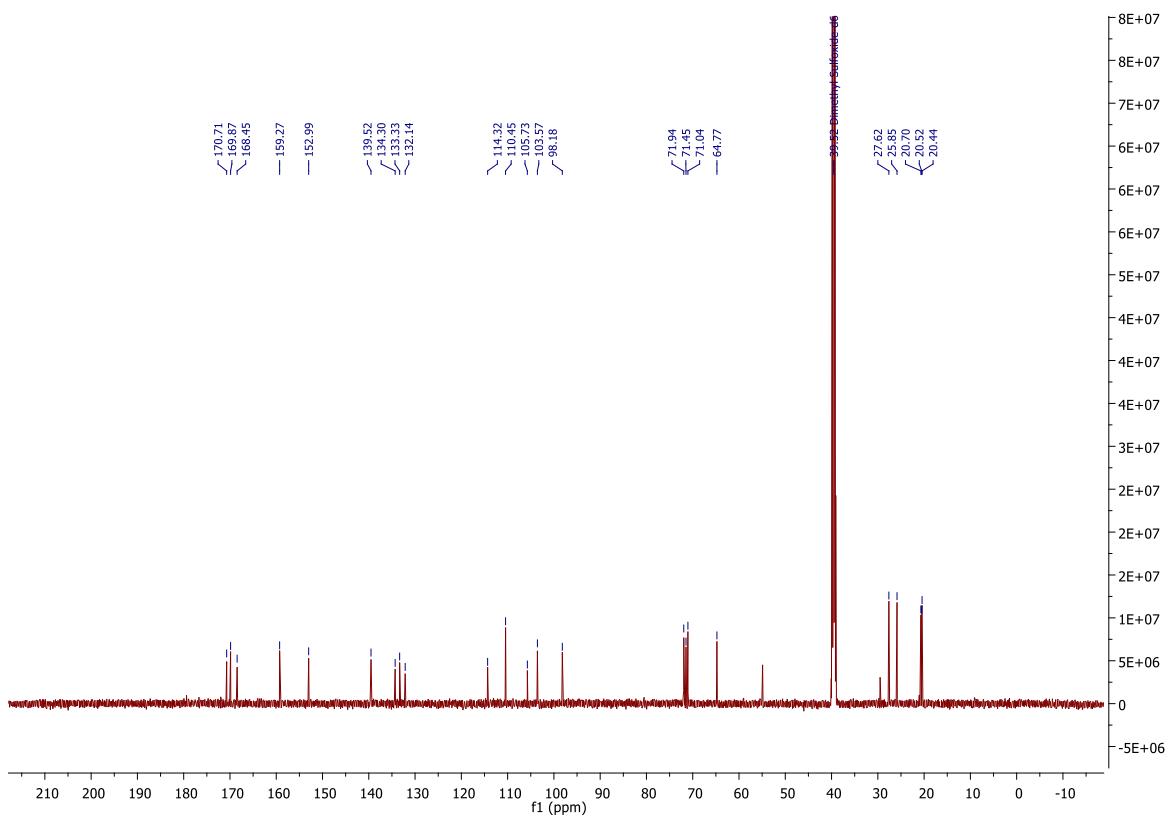


Figure S24. ^1H - ^{15}N HSQC of **24**

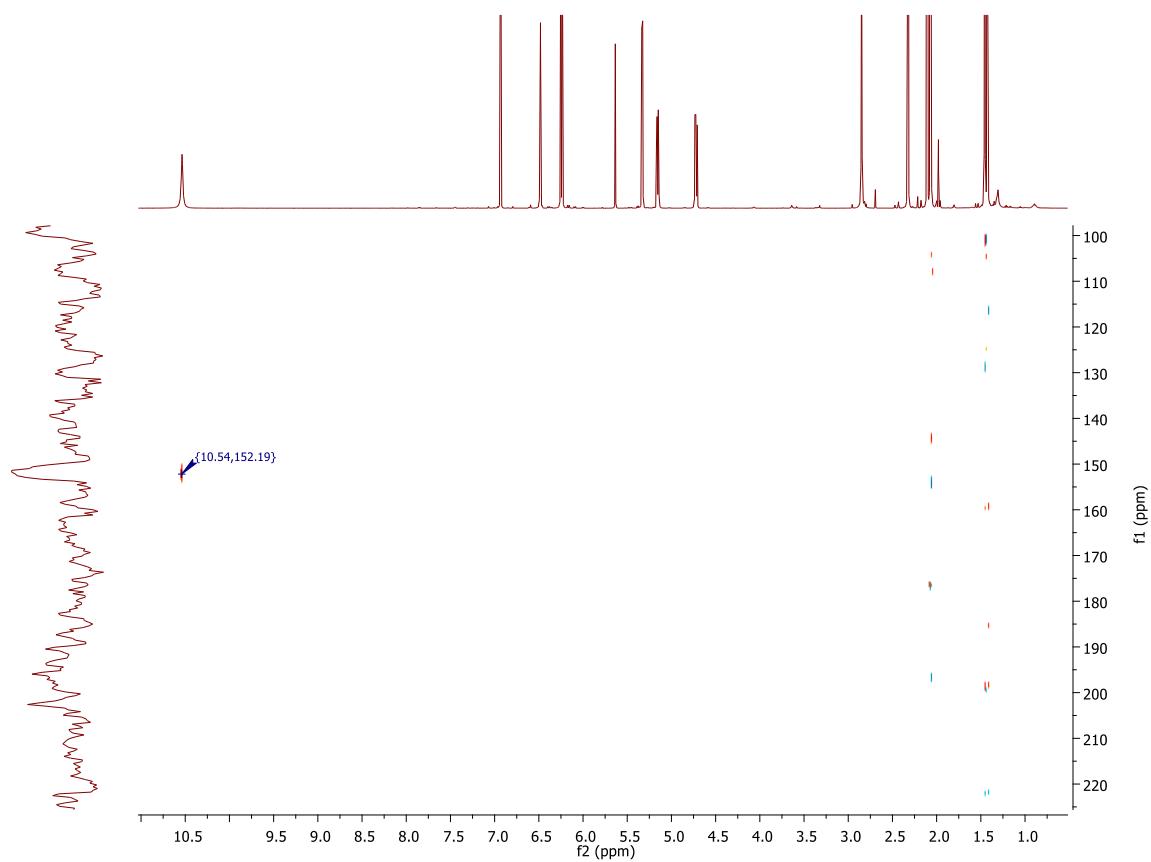


Figure S25. ^1H - ^{15}N HMBC of **24**

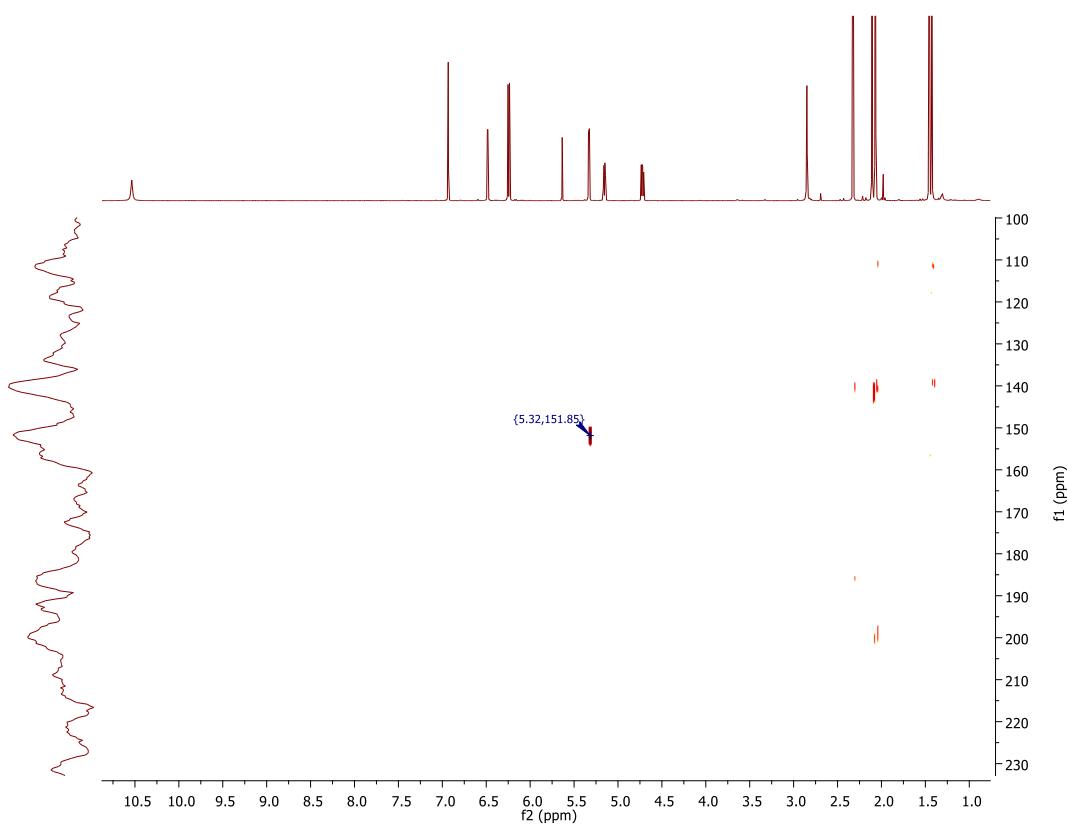


Figure S26. ^1H -NMR of 25

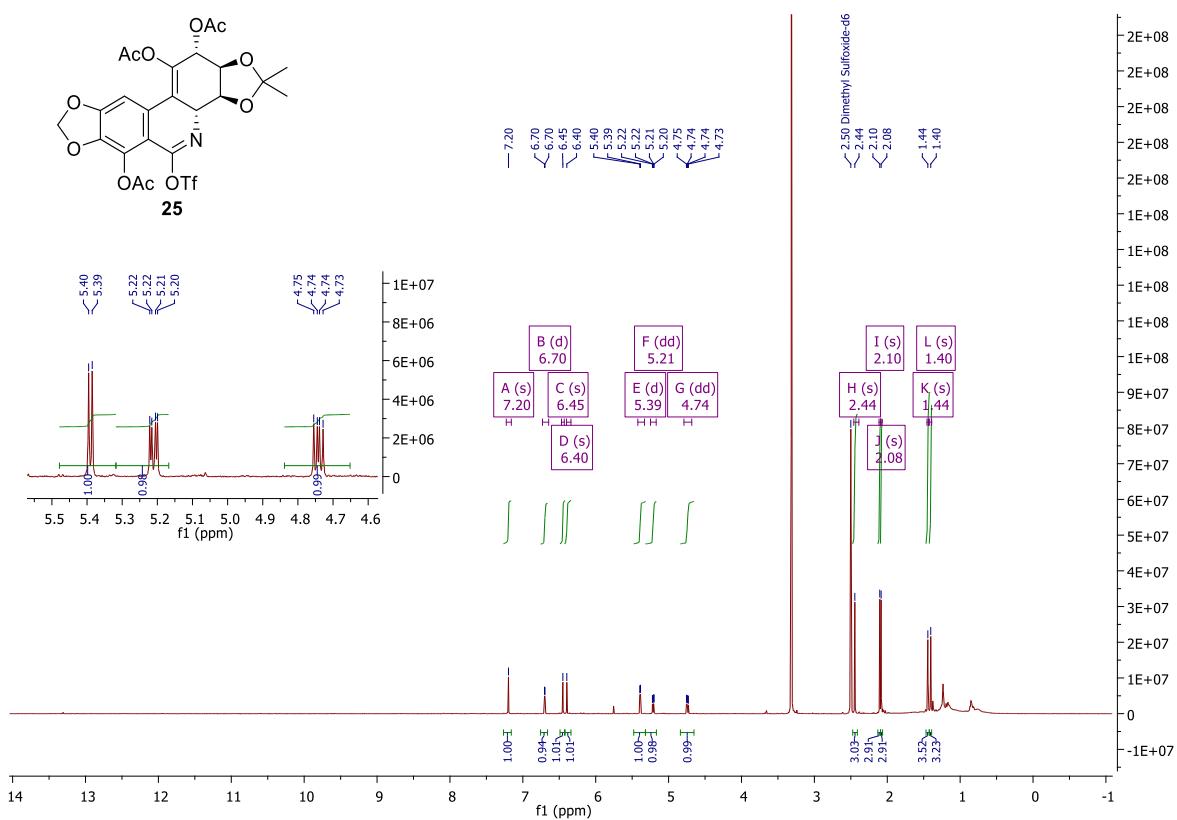


Figure S27. ^{13}C -NMR of 25

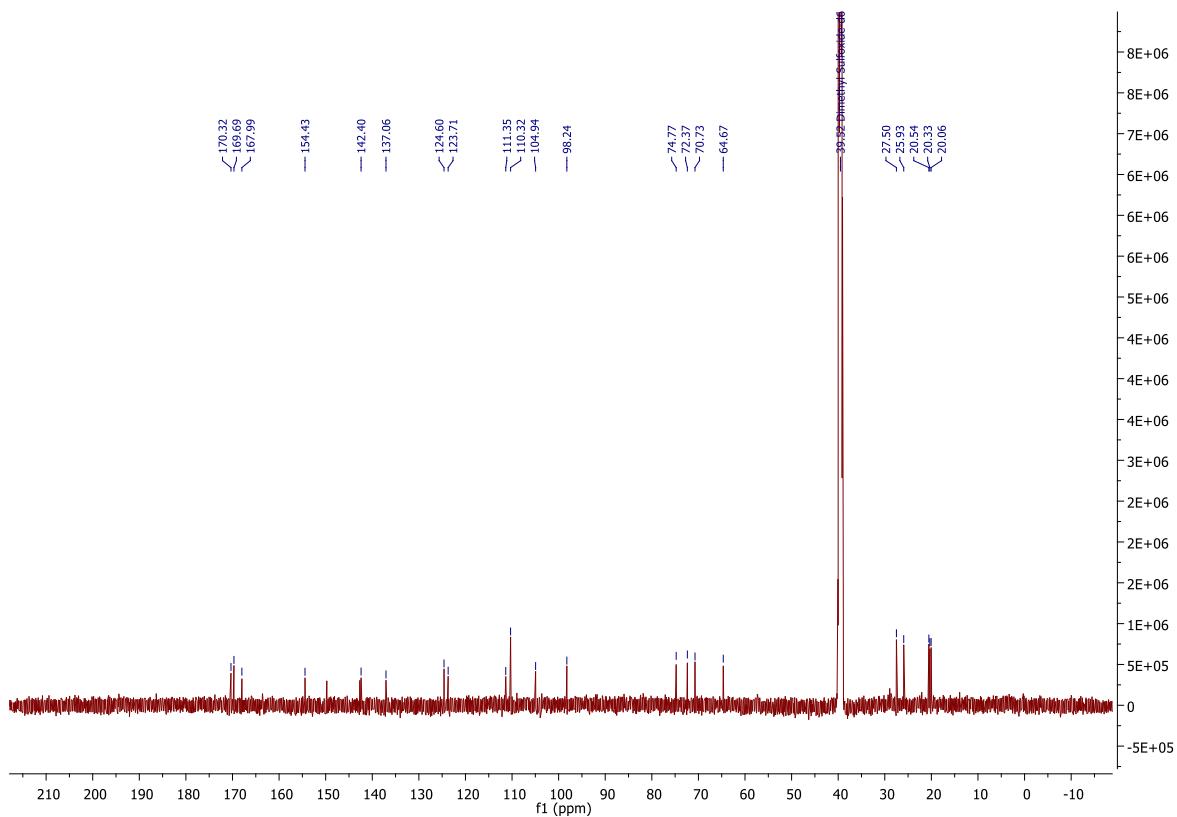


Figure S28. ^{19}F -NMR of **25**

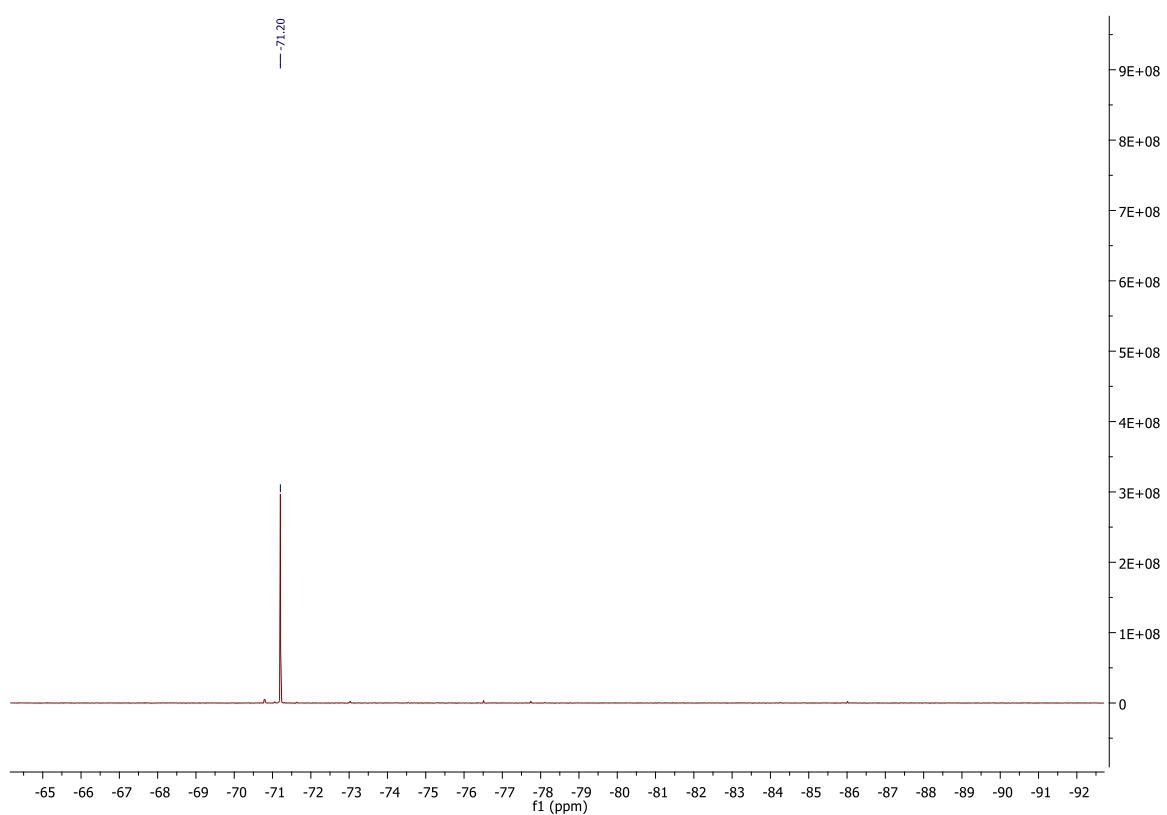


Figure S29. ^1H -NMR of **26**

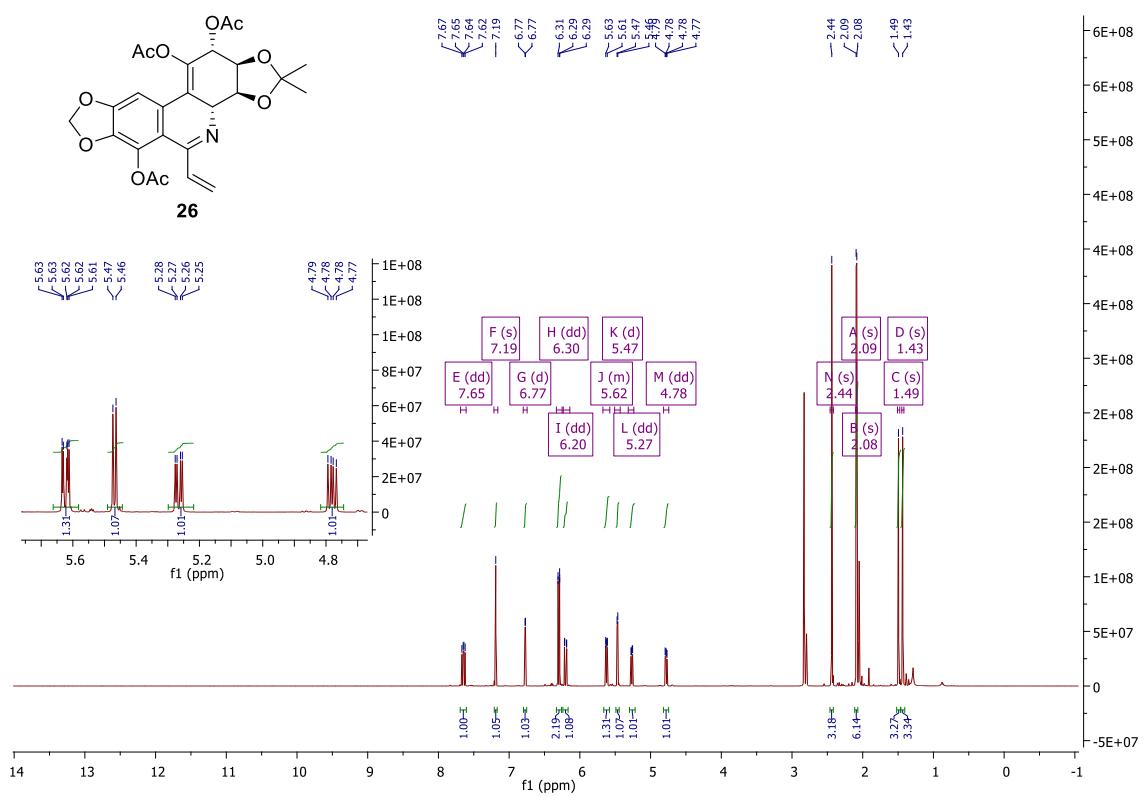


Figure S30. ^{13}C -NMR of **26**

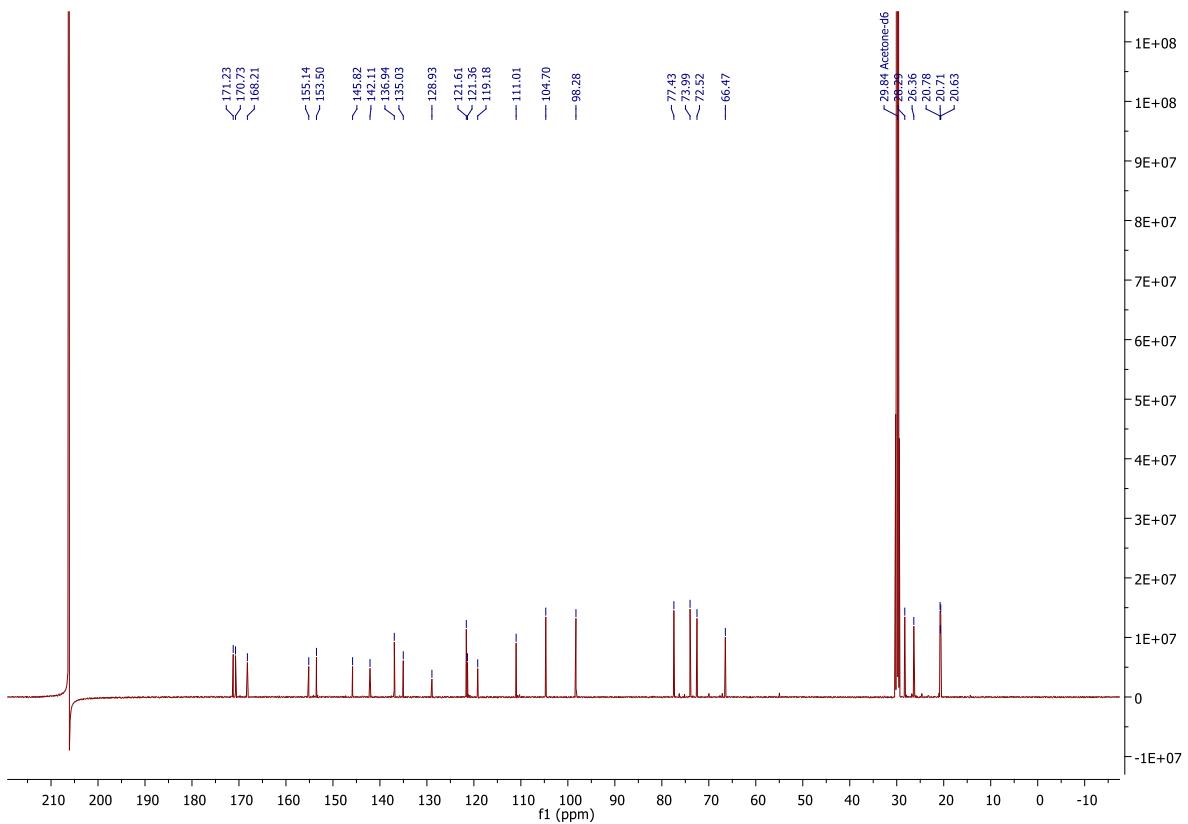


Figure S31. ^1H - ^{15}N HMBC of **26**

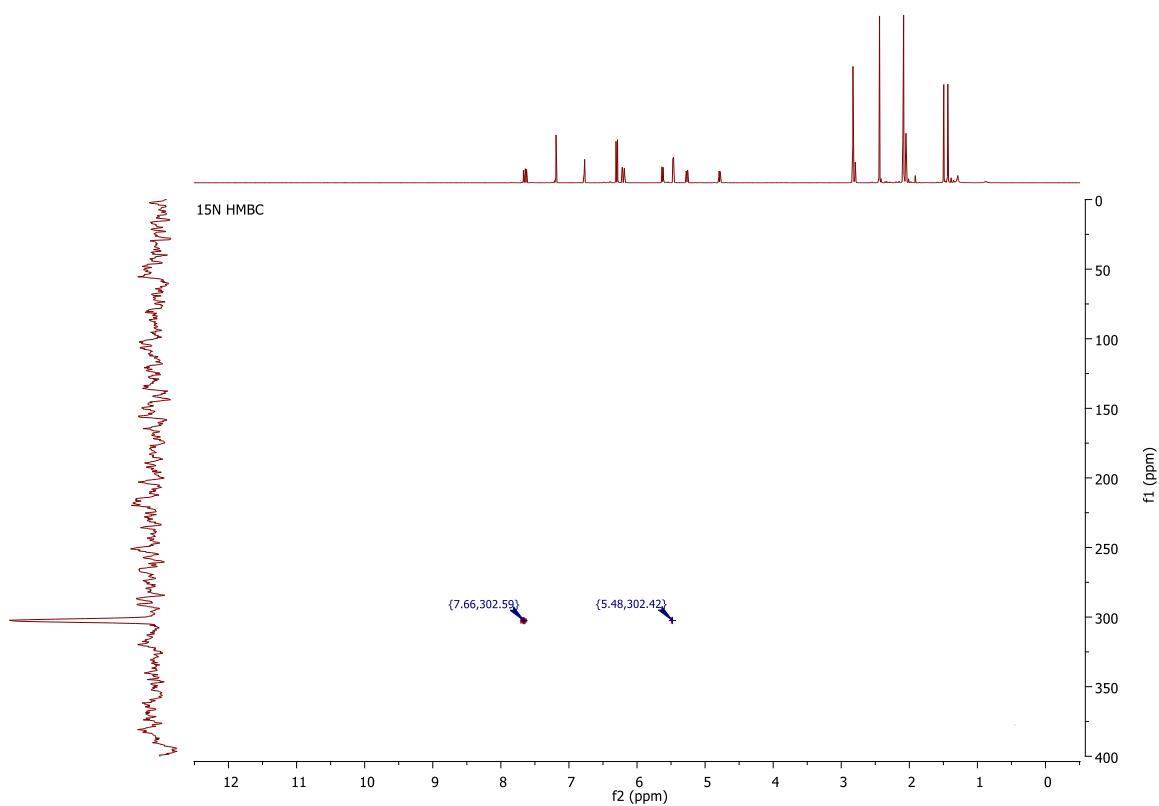


Figure S32. ^1H -NMR of **27**

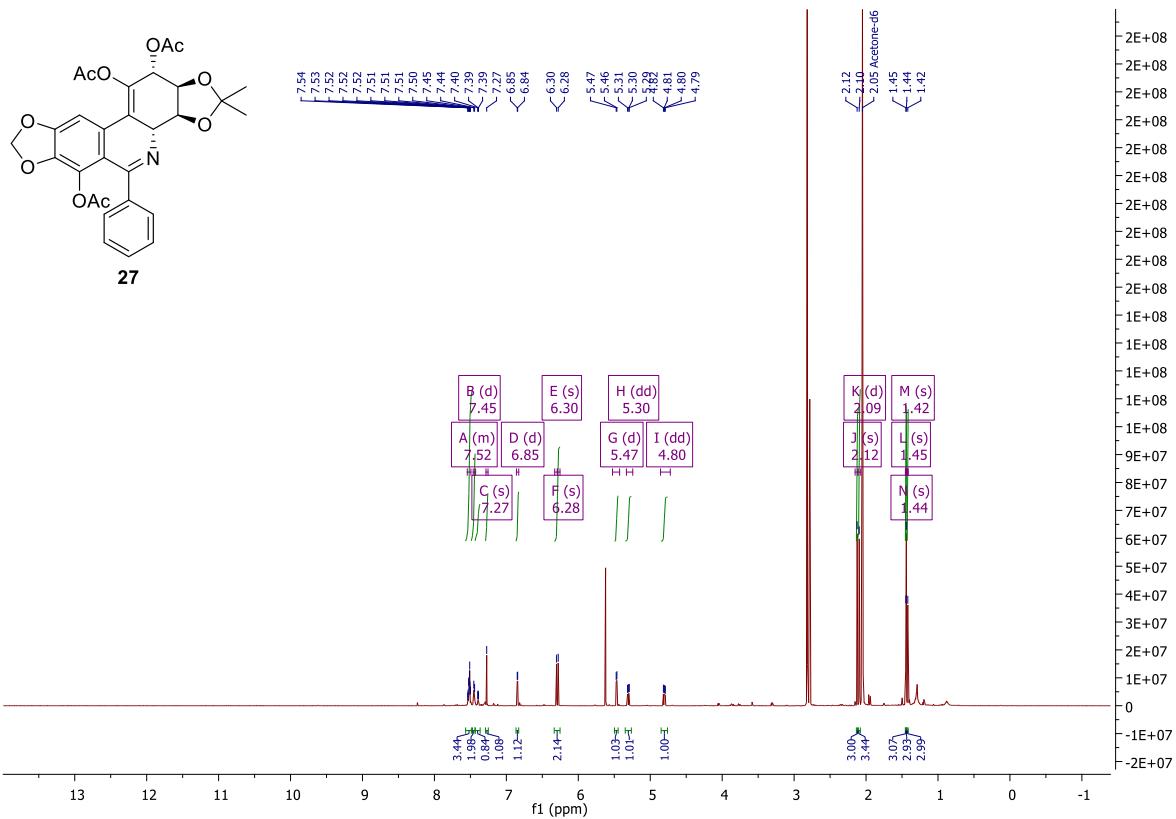


Figure S33. ^{13}C -NMR of 27

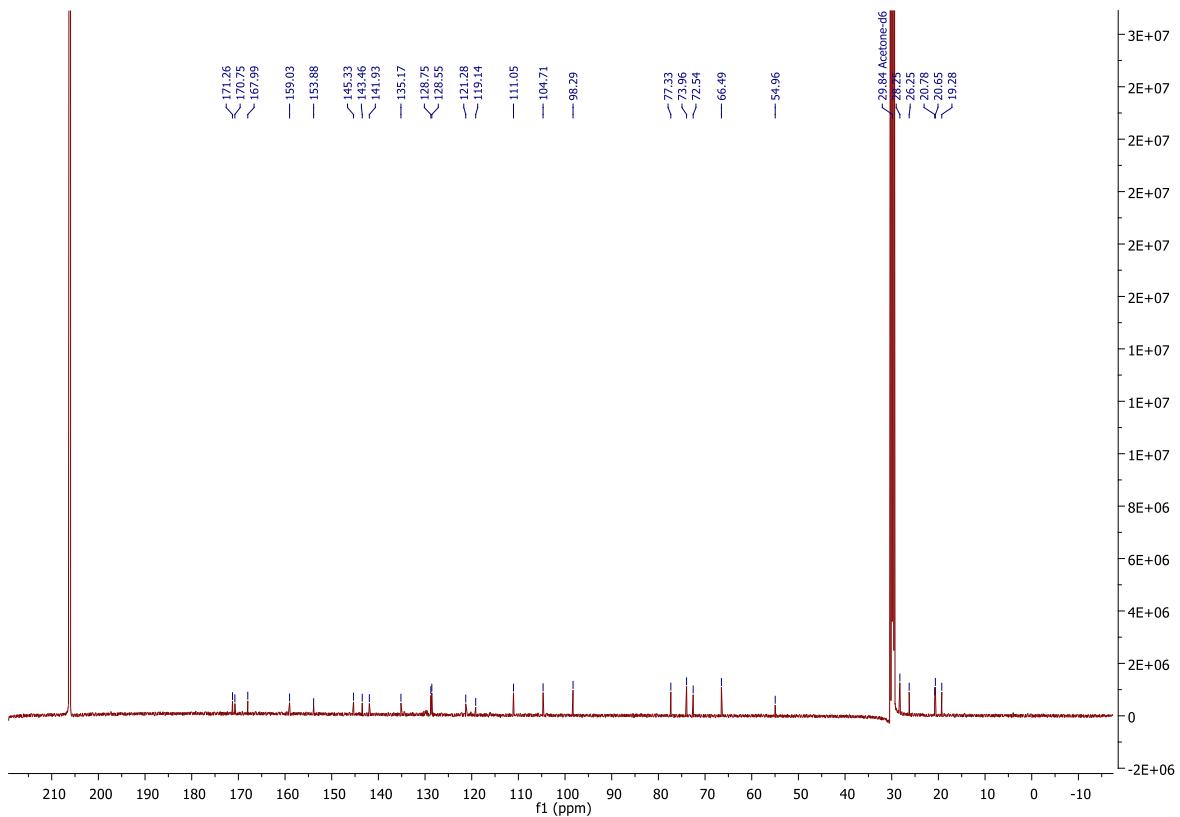


Figure S34. ^1H -NMR of **28**

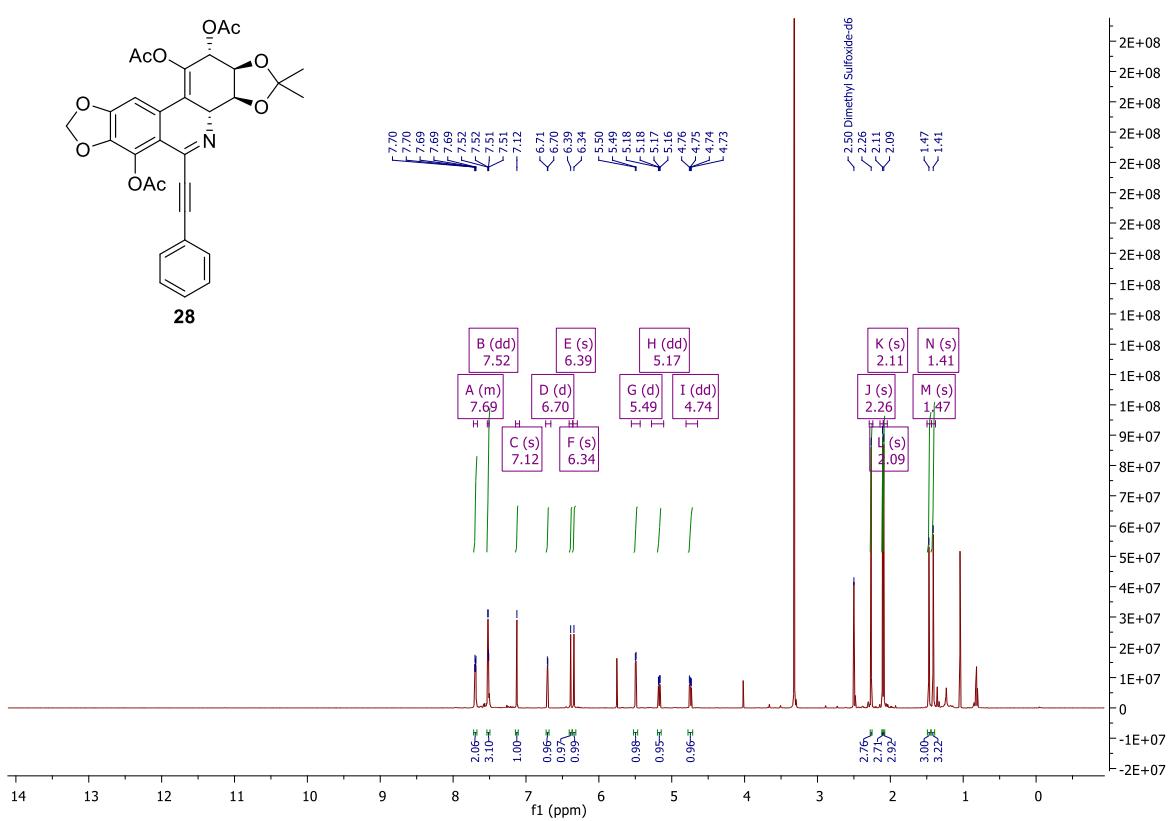


Figure S35. ^{13}C -NMR of **28**

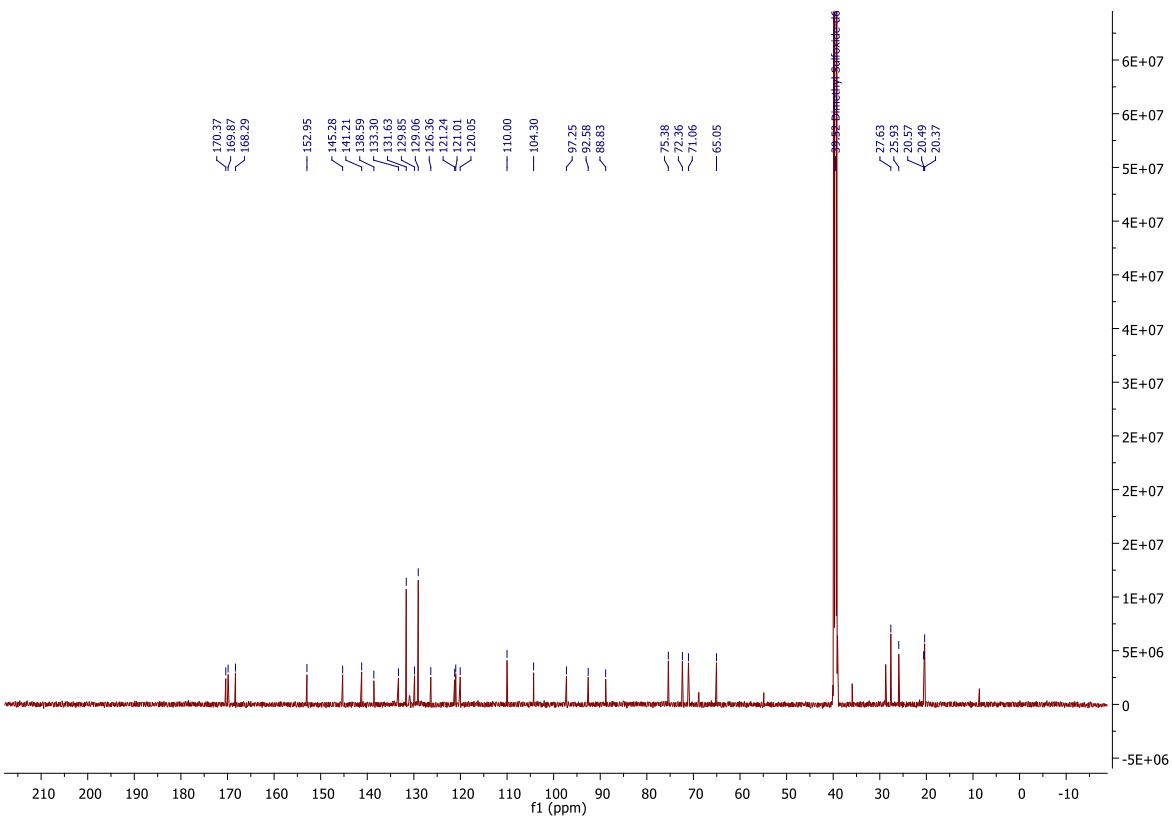


Figure S36. ^1H -NMR of **29**

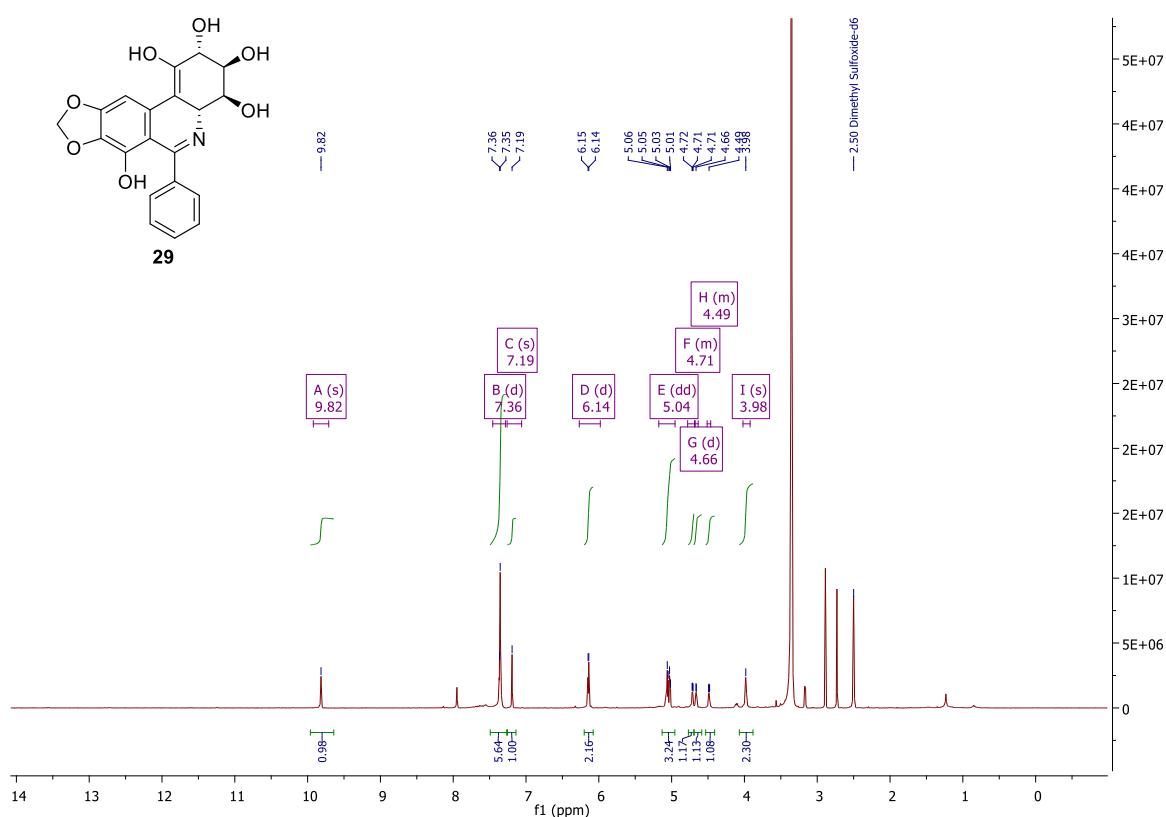


Figure S37. ^{13}C -NMR of **29**

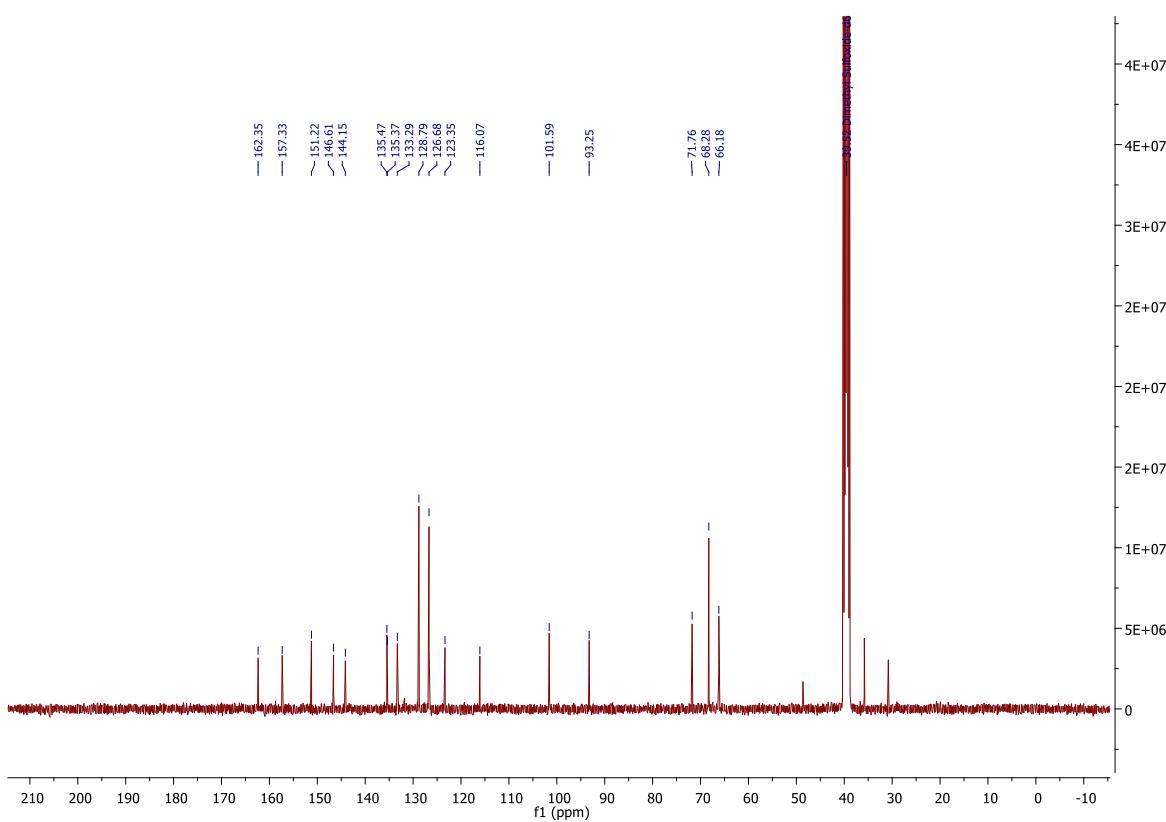


Figure S38. ^1H -NMR of **30**

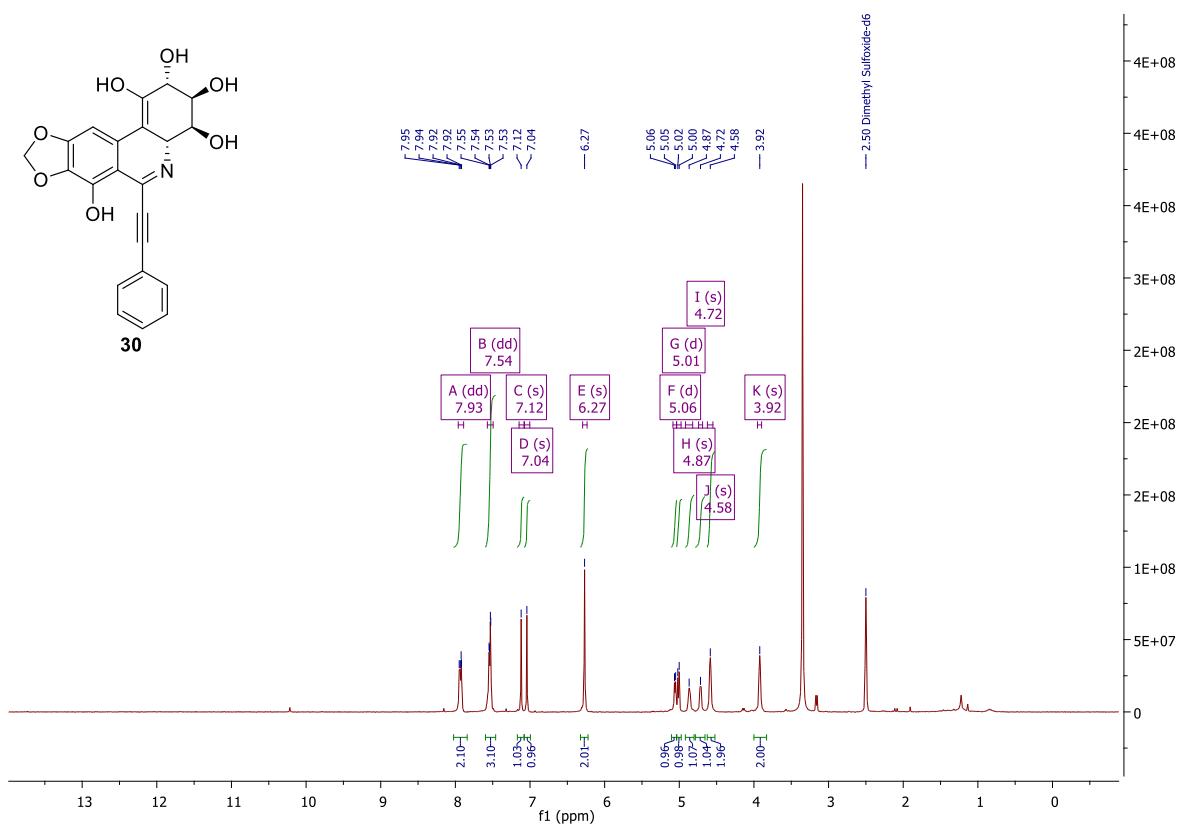


Figure S39. ^{13}C -NMR of **30**

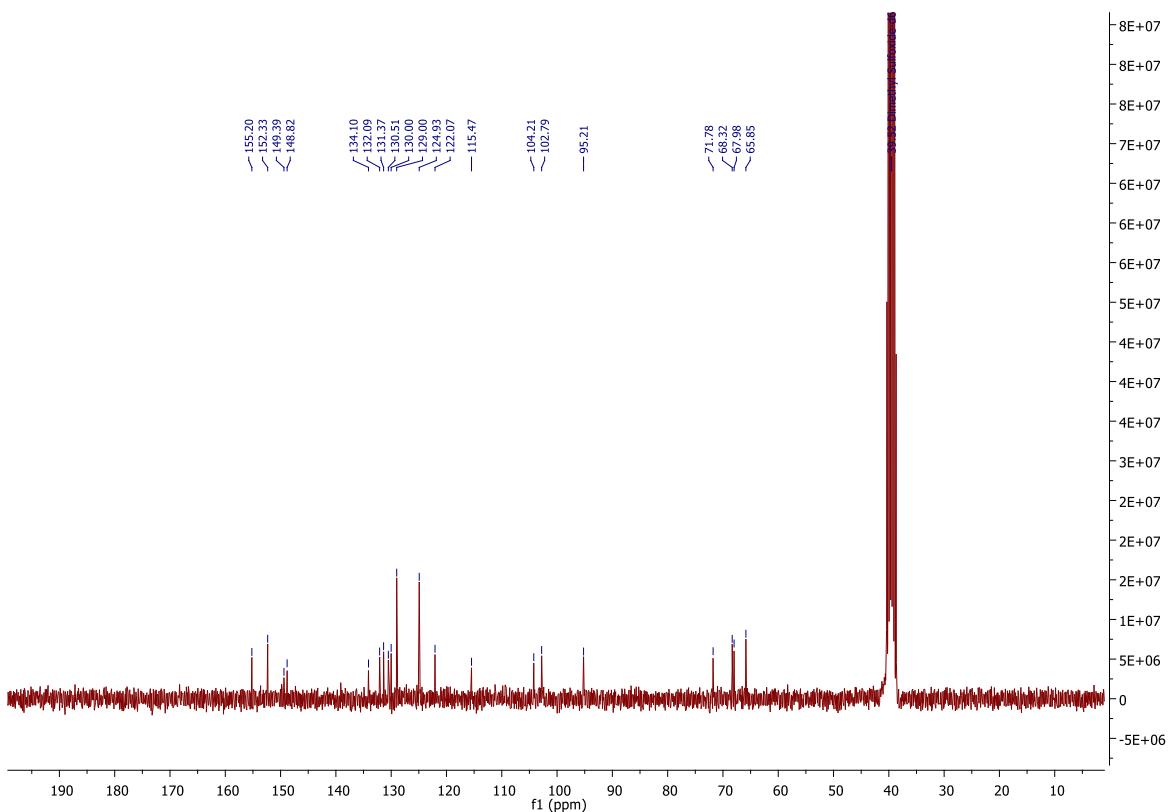


Figure S40. ^1H -NMR of **31**

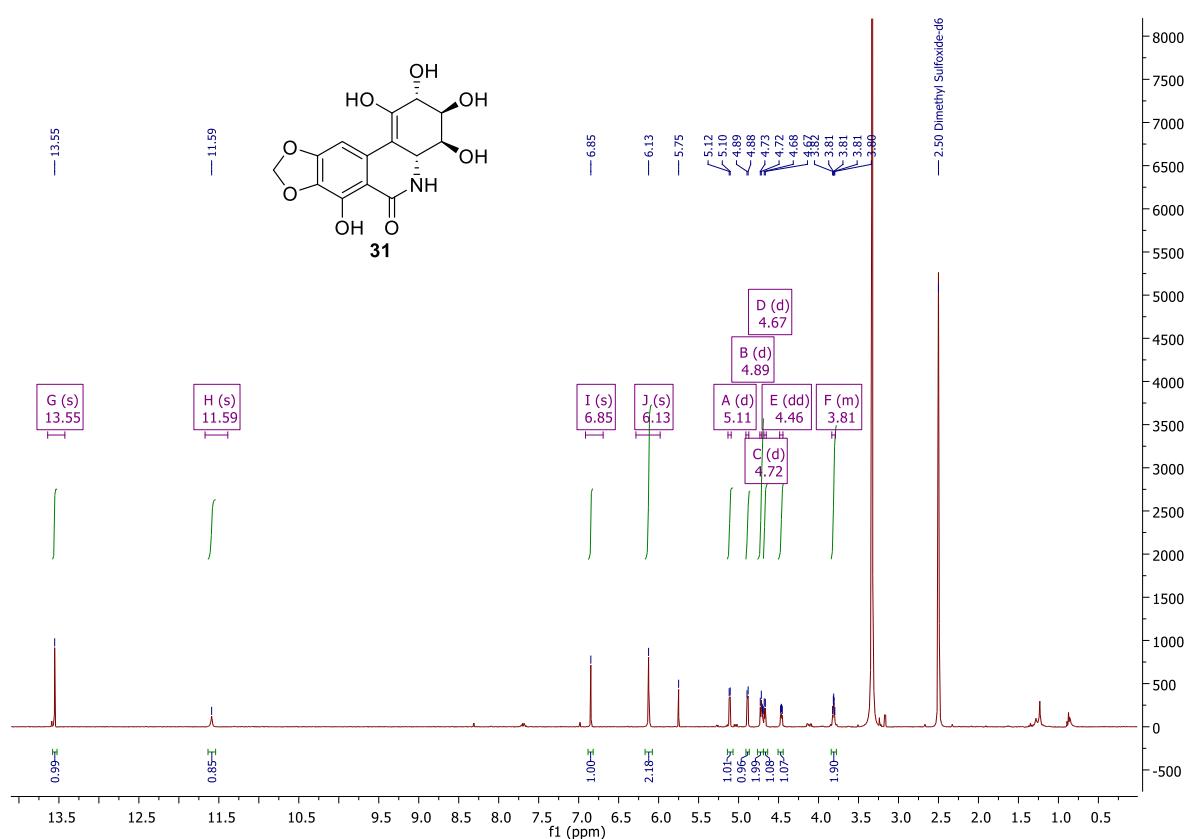


Figure S41. ^{13}C -NMR of **31**

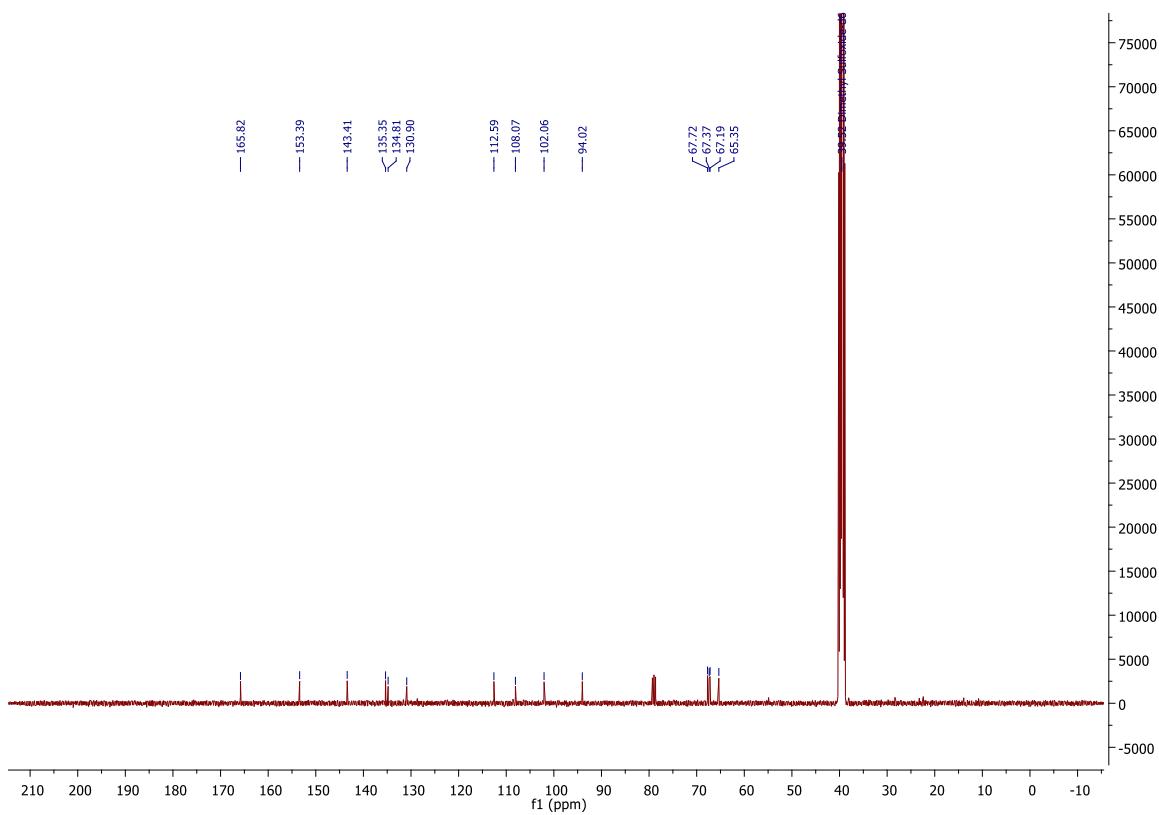


Figure S42. ^1H -NMR of 33

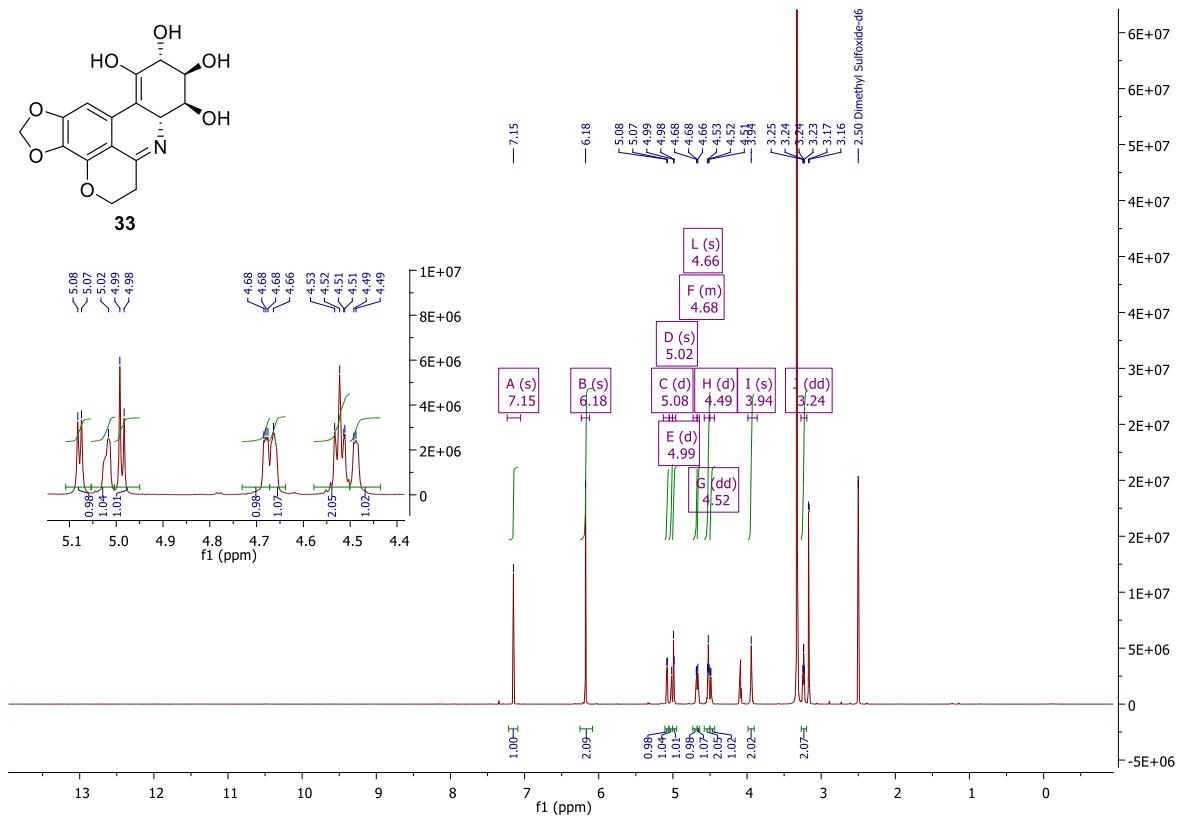


Figure S43. ^{13}C -NMR of 33

