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Supplemental Material to:

Synthesis and pharmacological in-vitro investigations of novel shikonin derivatives with a special focus on cyclopropane bearing derivatives

Nadine Kretschmer [1], Antje Hufner [2], Christin Durchschein [1], Katrin Popodi [1], Beate Rinner [3], Birgit Lohberger [4], Rudolf Bauer [1*]

[1] Institute of Pharmaceutical Sciences, Department of Pharmacognosy, University of Graz, Beethovenstr. 8, 8010 Graz, Austria; nadine.kretschmer@uni-graz.at (N.K.); christin.durchschein@hotmail.com (C.D.); katrin.popodi@gmx.at (K.P.)
[2] Institute of Pharmaceutical Sciences, Department of Pharmaceutical Chemistry, University of Graz, Universitaetsplatz 1, 8010 Graz, Austria; antje.huefner@uni-graz.at (A.H.)
[3] Division of Biomedical Research, Medical University of Graz, Roseggerweg 48, 8036 Graz, Austria; beate.rinner@medunigraz.at (B.R.)
[4] Department of Orthopedics and Trauma, Medical University Graz, Auenbruggerplatz 5, 8036 Graz, Austria; birgit.lohberger@medunigraz.at (B.L.)
* Correspondence: rudolf.bauer@uni-graz.at (R.B.)

Content of supporting information file:

1. Results of XTT screening.

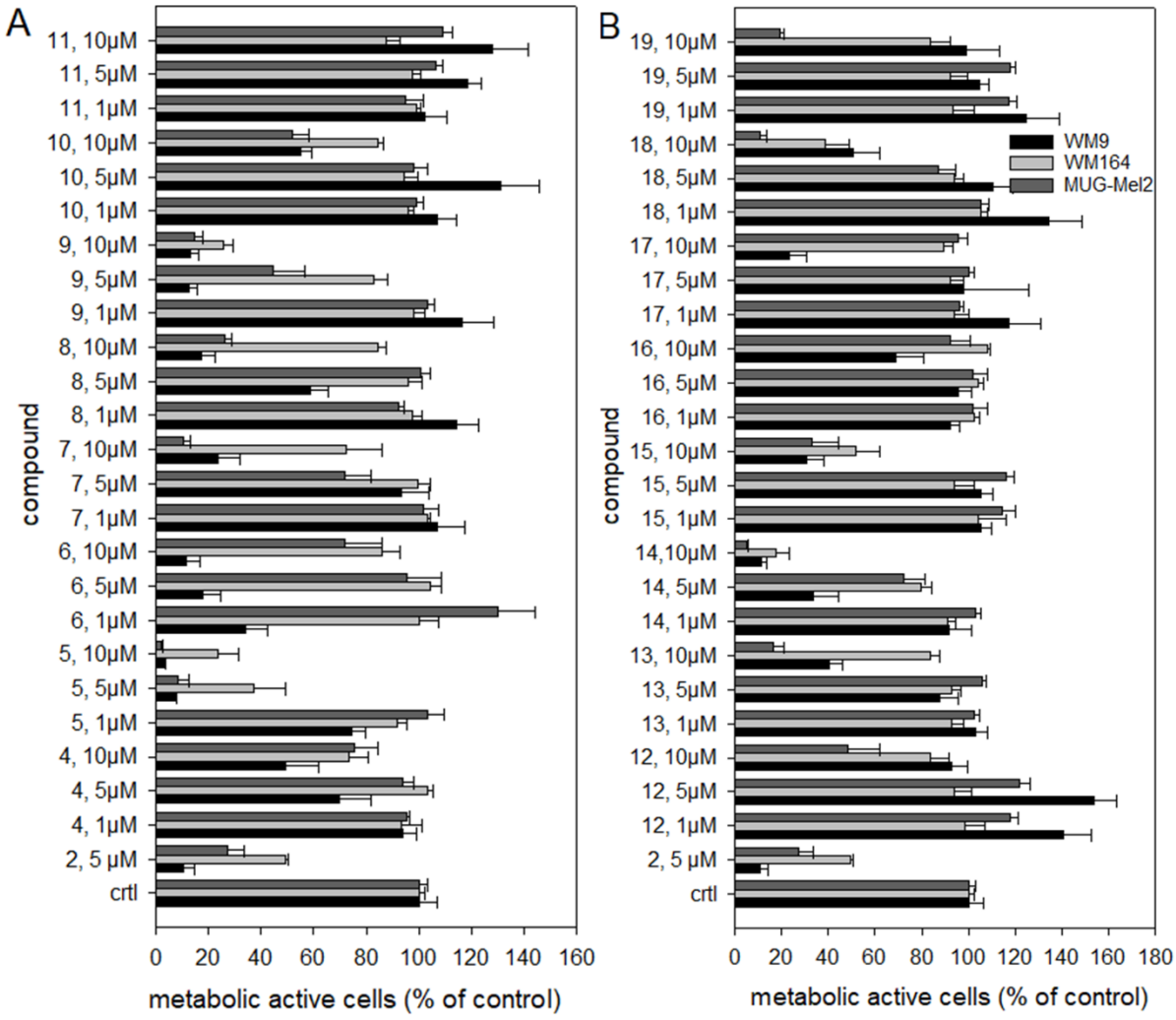


Figure S1. Results of compounds **4**-**11** (A) and to **12**-**19** (B) compared to 5.0 µM of **2**. Vinblastine was used as positive control. At a concentration of 0.01 nM, it reduced the cell viability compared to control cells to: WM9 cells: 23.8 ± 1.5 %, WM164 cells: 59.4 ± 4.4 %, and MUG-Mel2 cells: 65.0 ± 6.9 % (n = 6, mean ± sem, 72h of treatment).

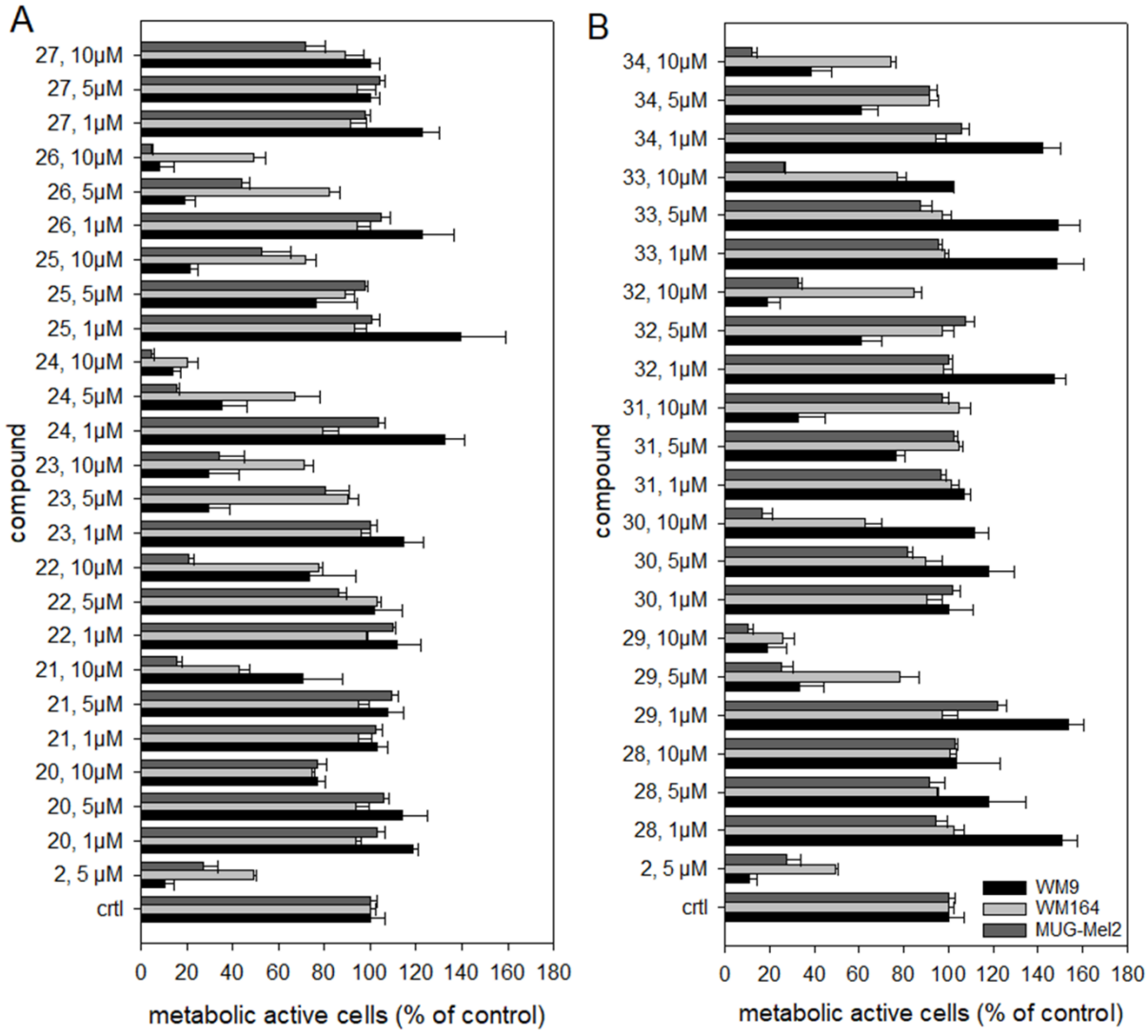
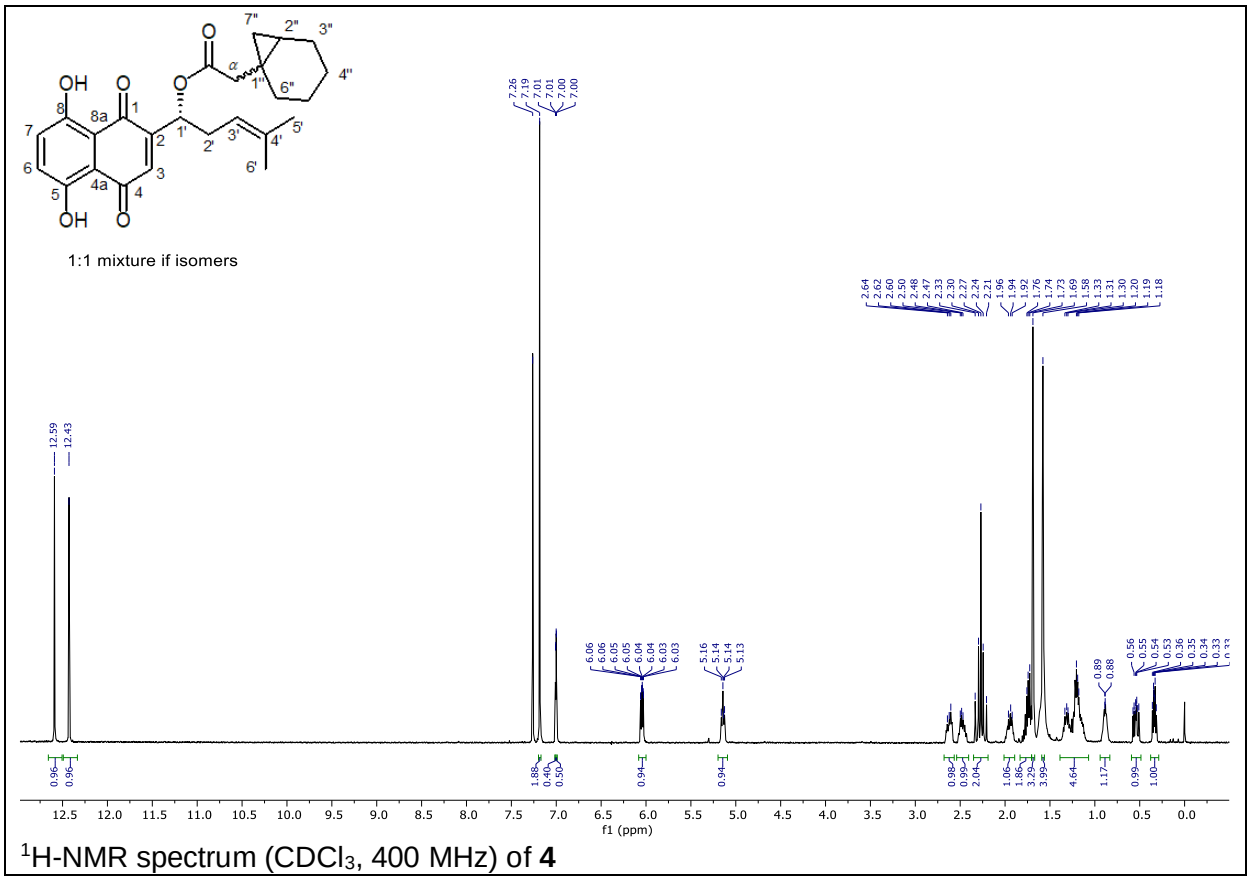
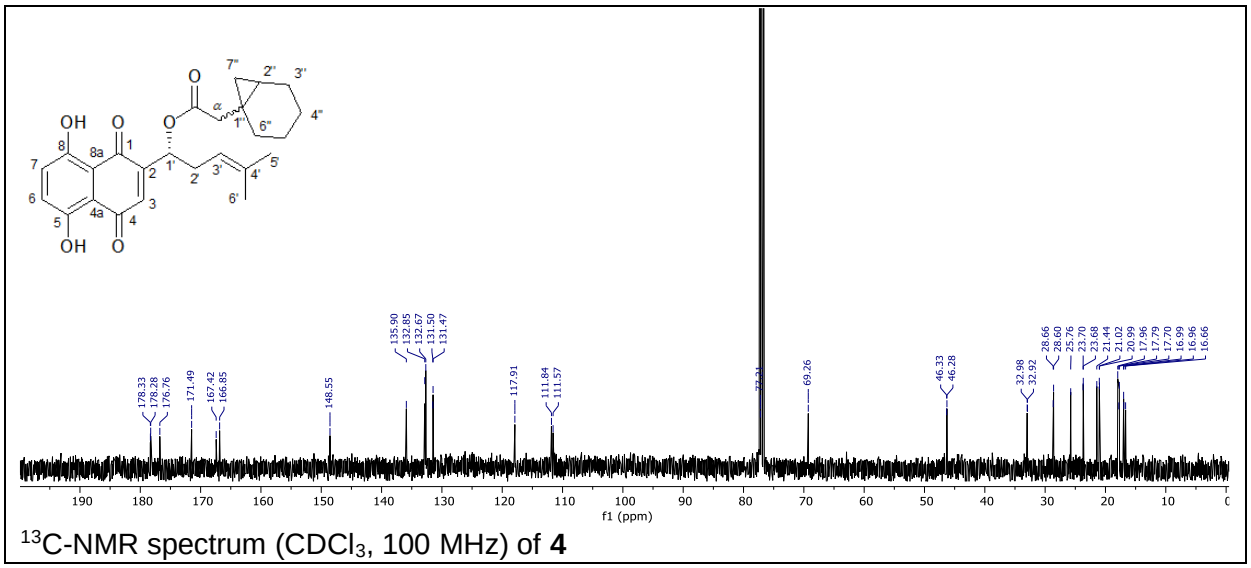


Figure S2. Results of compounds **20**-**27** (A) and **28**-**34** (B) compared to 5.0 µM of **2**. Vinblastine was used as positive control. At a concentration of 0.01 nM, it reduced the cell viability compared to control cells to: WM9 cells: 23.8 ± 1.5 %, WM164 cells: 59.4 ± 4.4 %, and MUG-Mel2 cells: 65.0 ± 6.9 % (n = 6, mean ± sem, 72h of treatment).

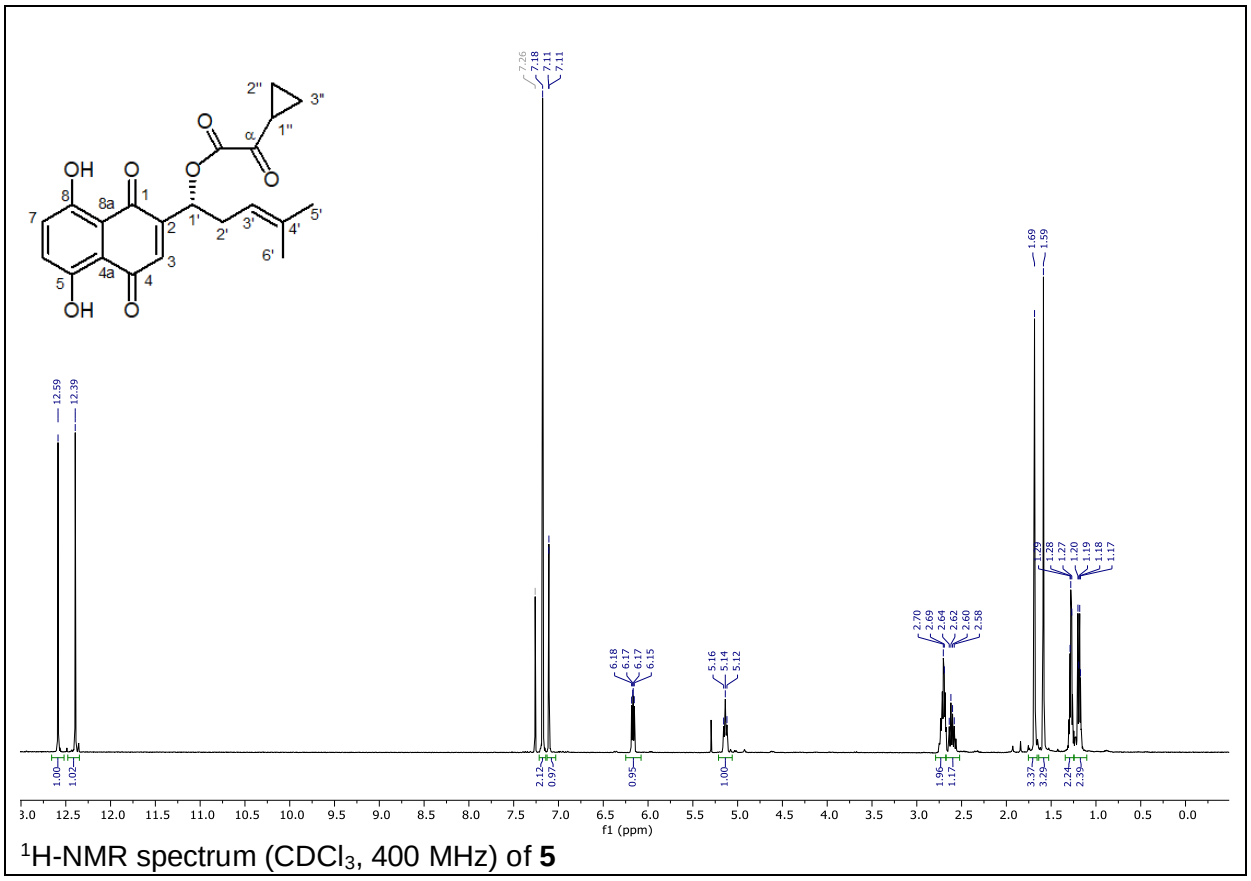
2. ^{1}H-NMR spectra ($CDCl_3$, 400 MHz) of all shikonin derivatives synthesized for this study and ^{13}C-NMR spectra (100 MHz) or HMBC spectra of derivatives with yet unknown ^{13}C-NMR spectra



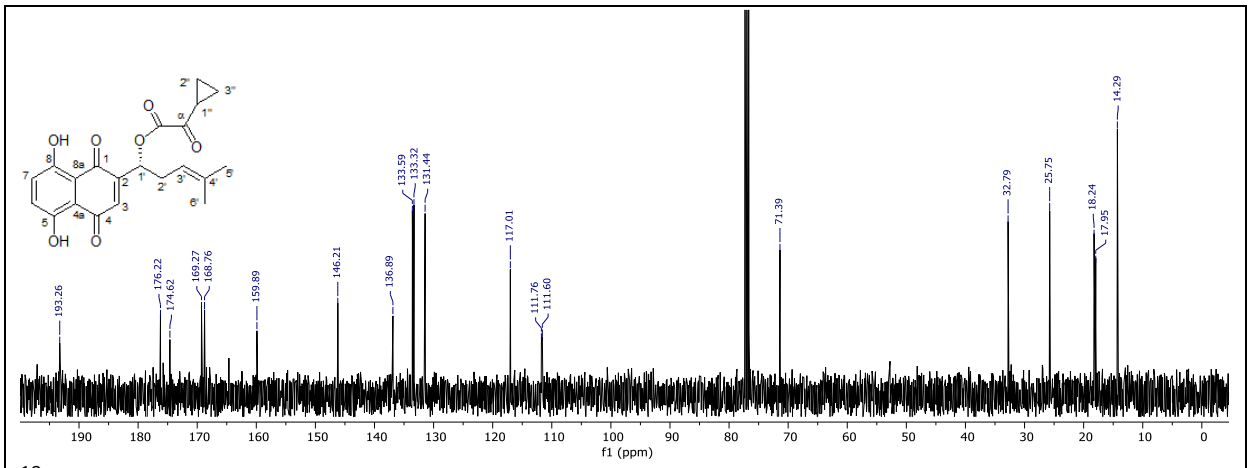
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **4**



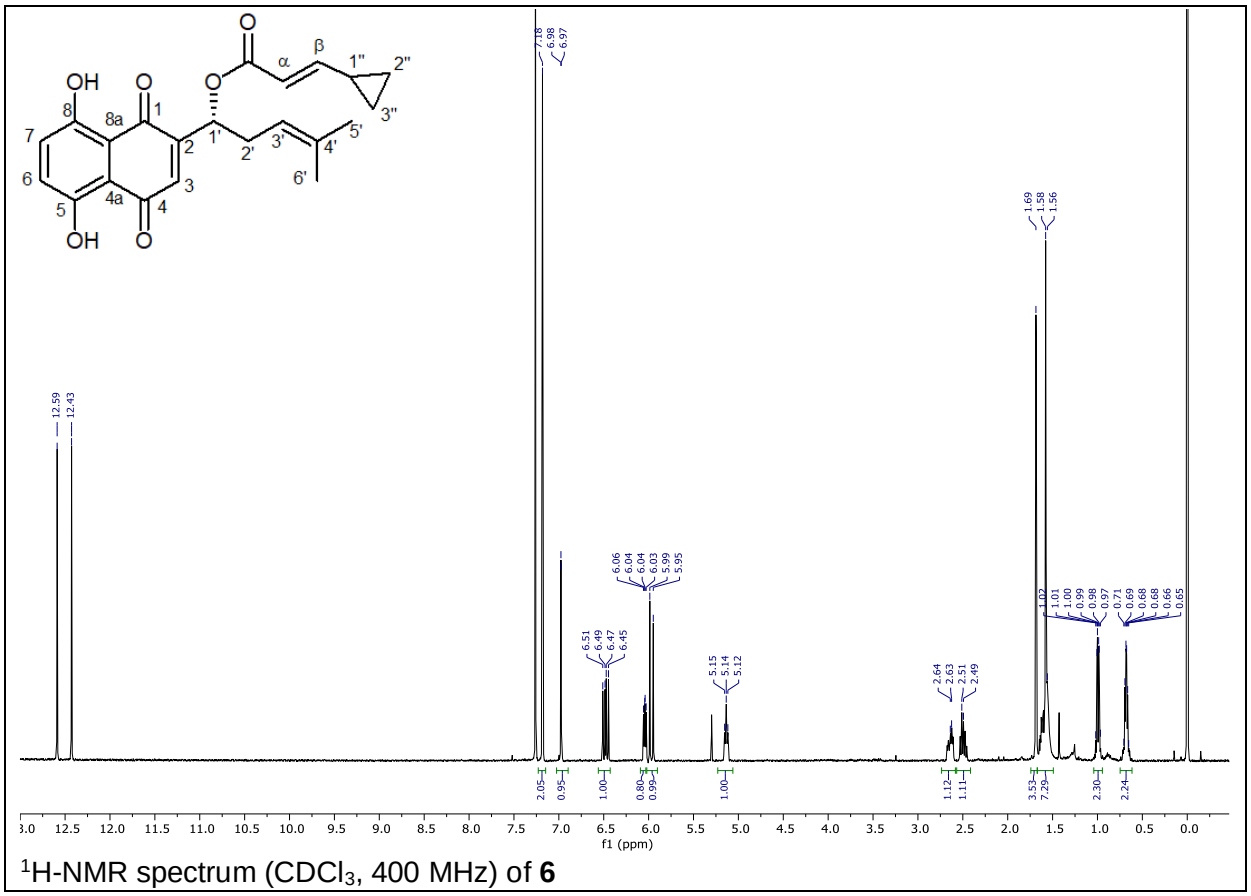
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **4**



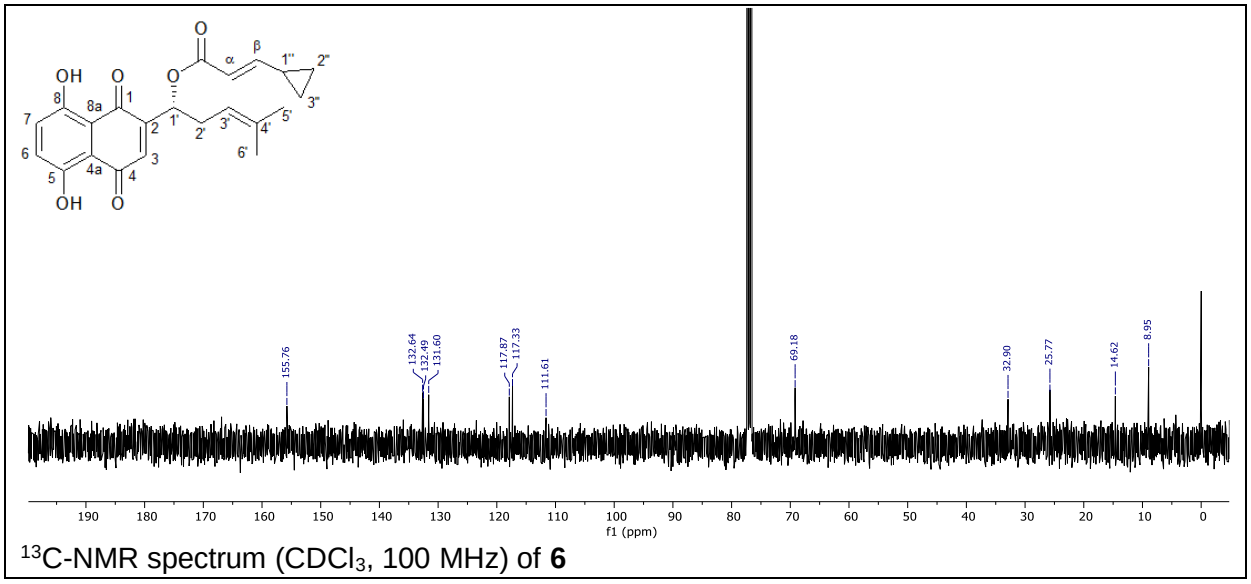
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **5**



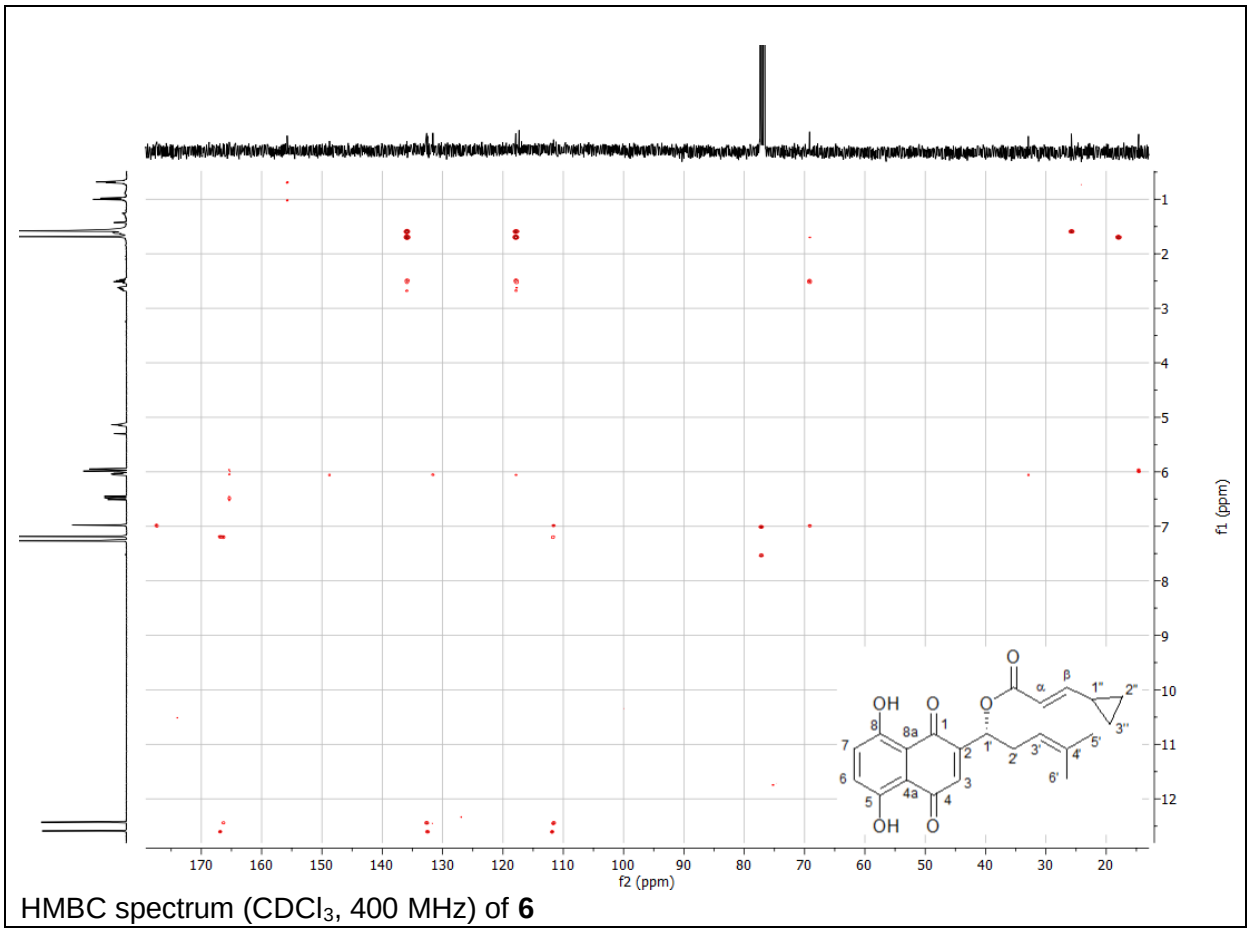
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **5**



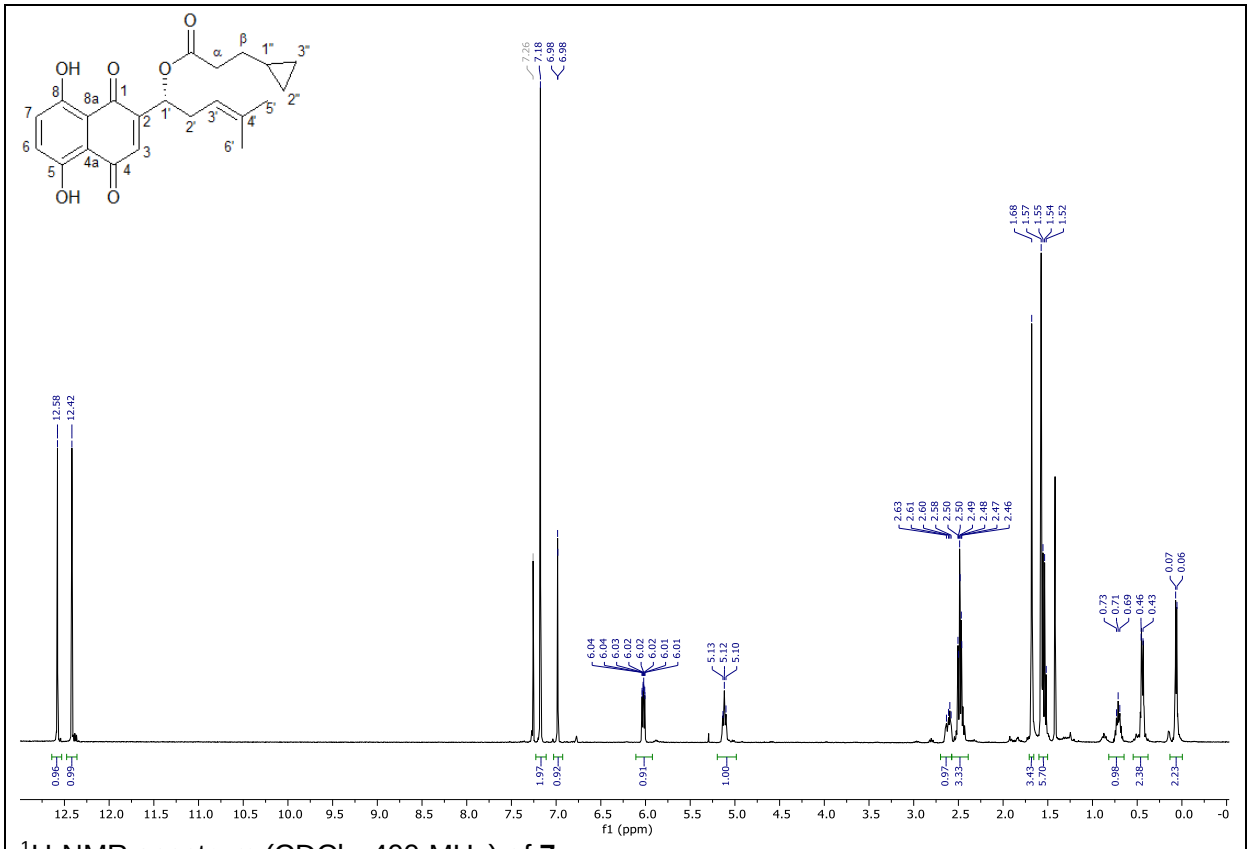
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **6**



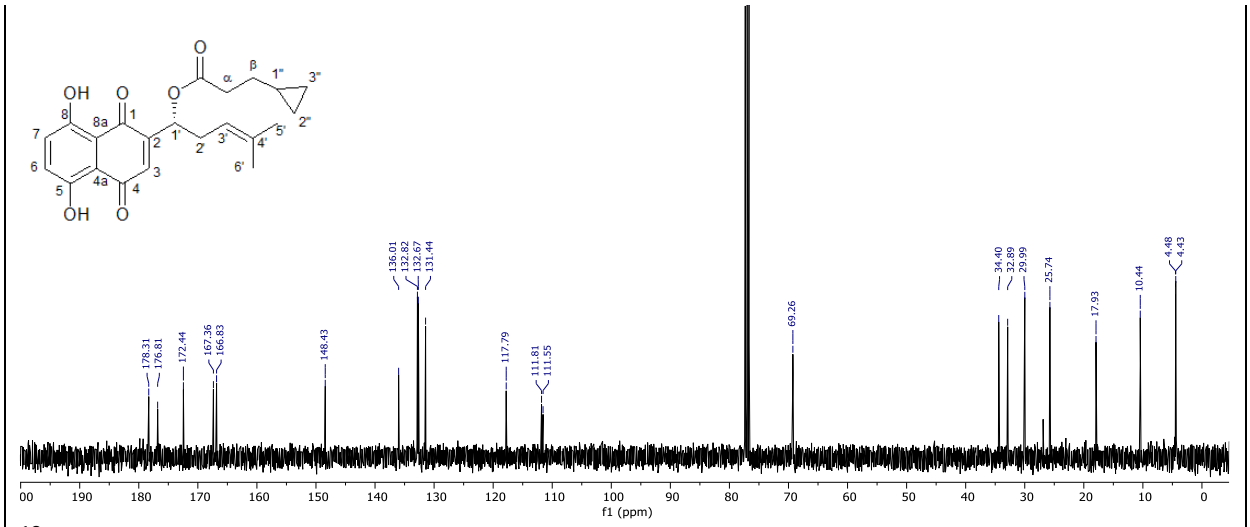
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **6**



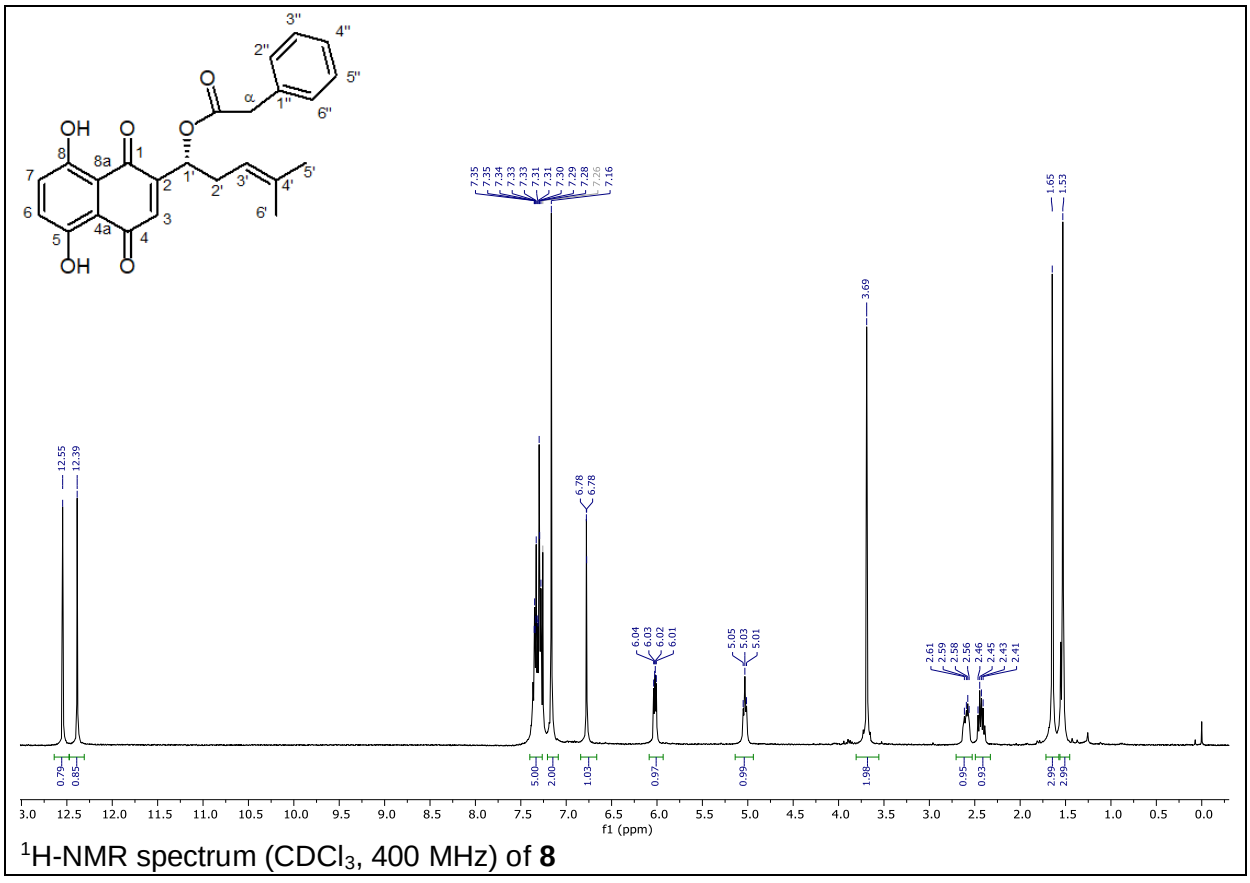
HMBC spectrum ($CDCl_3$, 400 MHz) of **6**



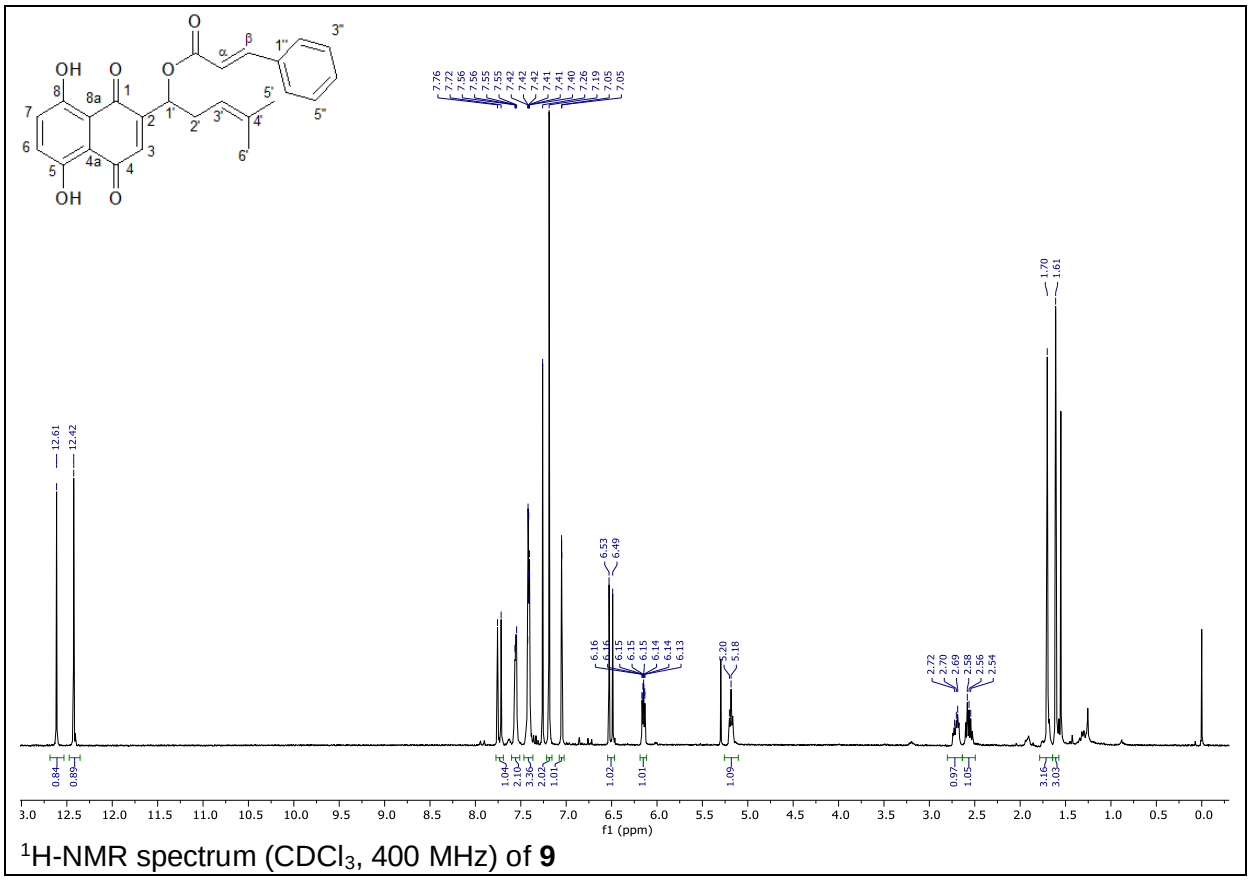
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **7**



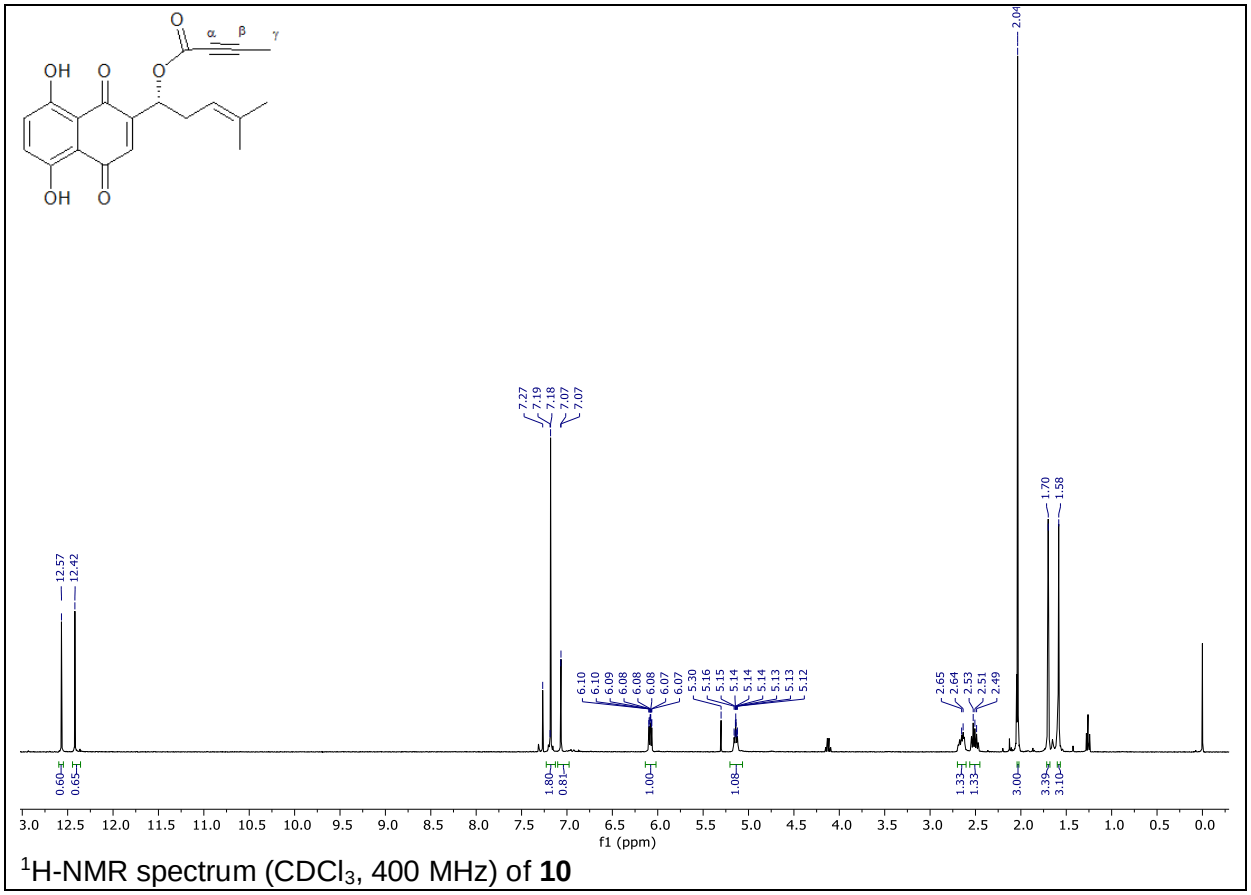
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **7**



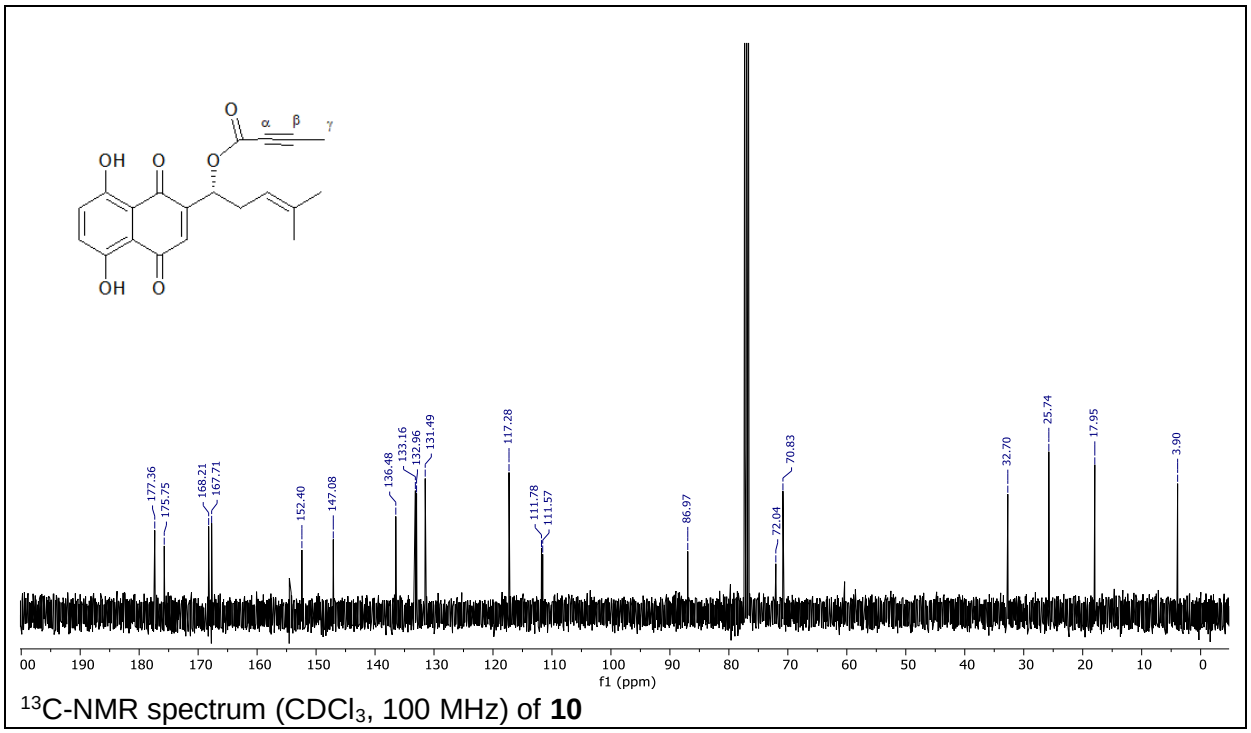
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **8**



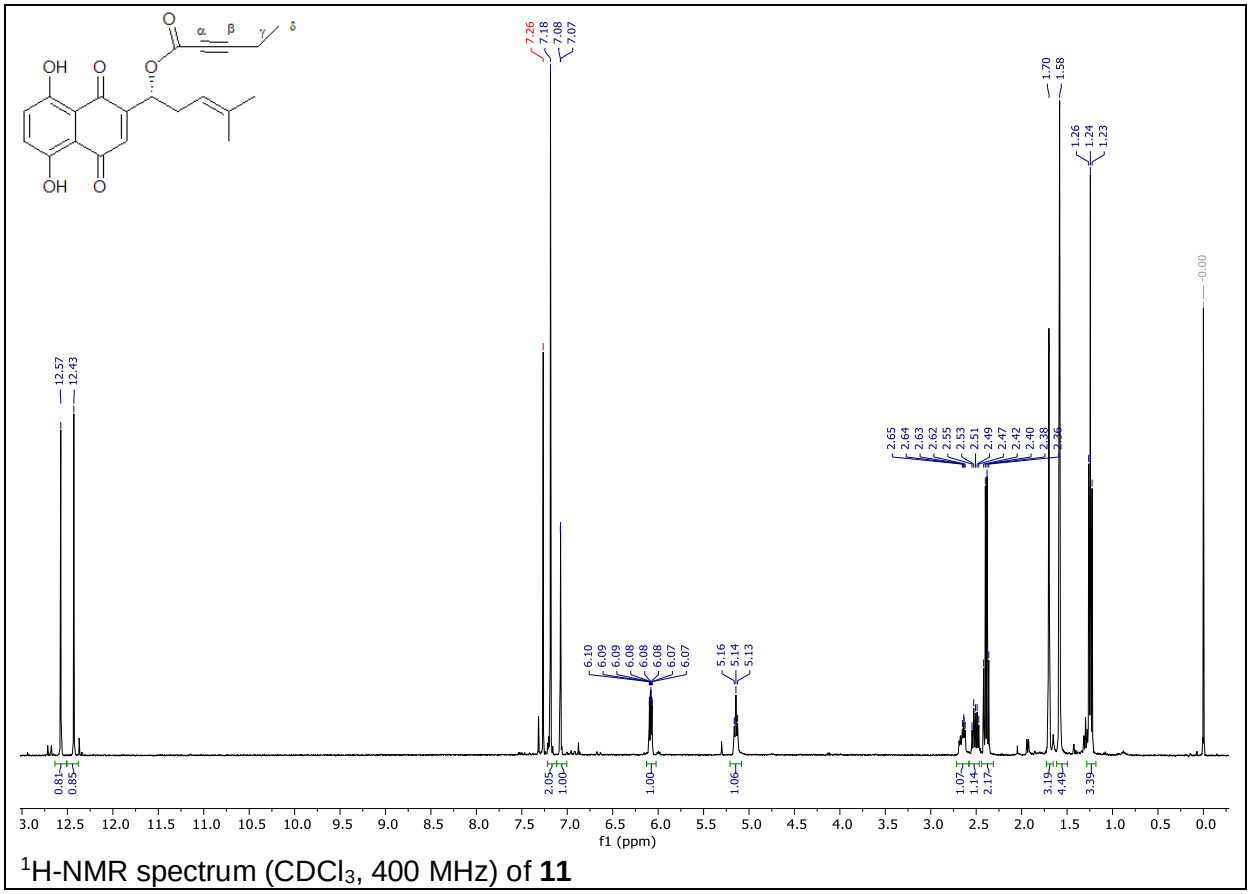
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **9**



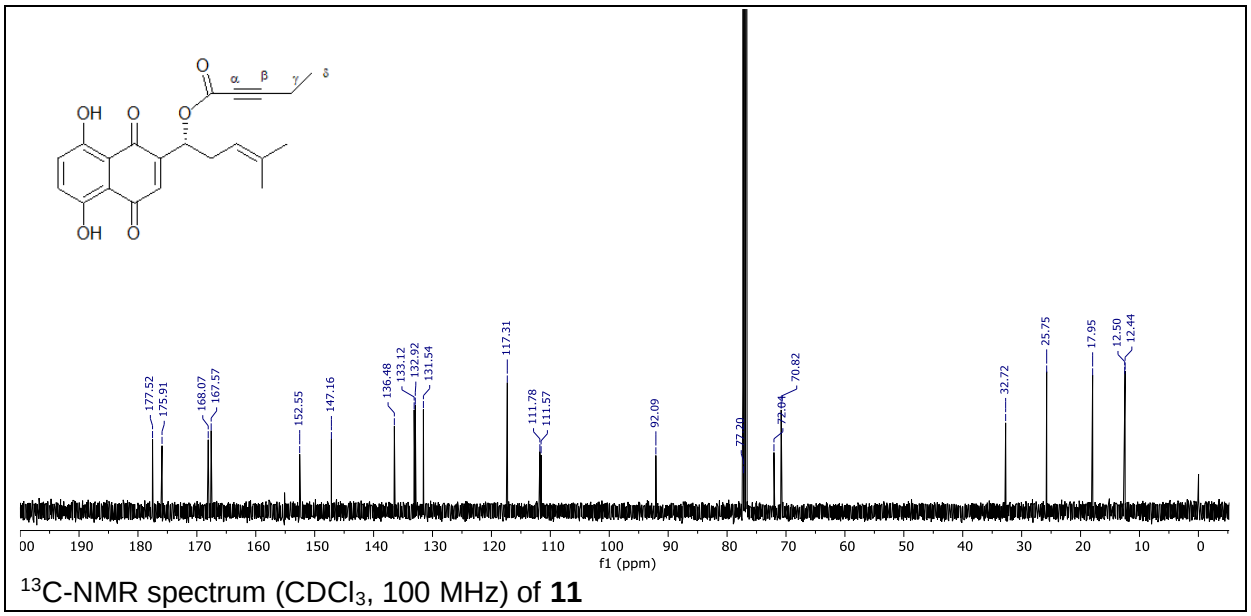
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **10**



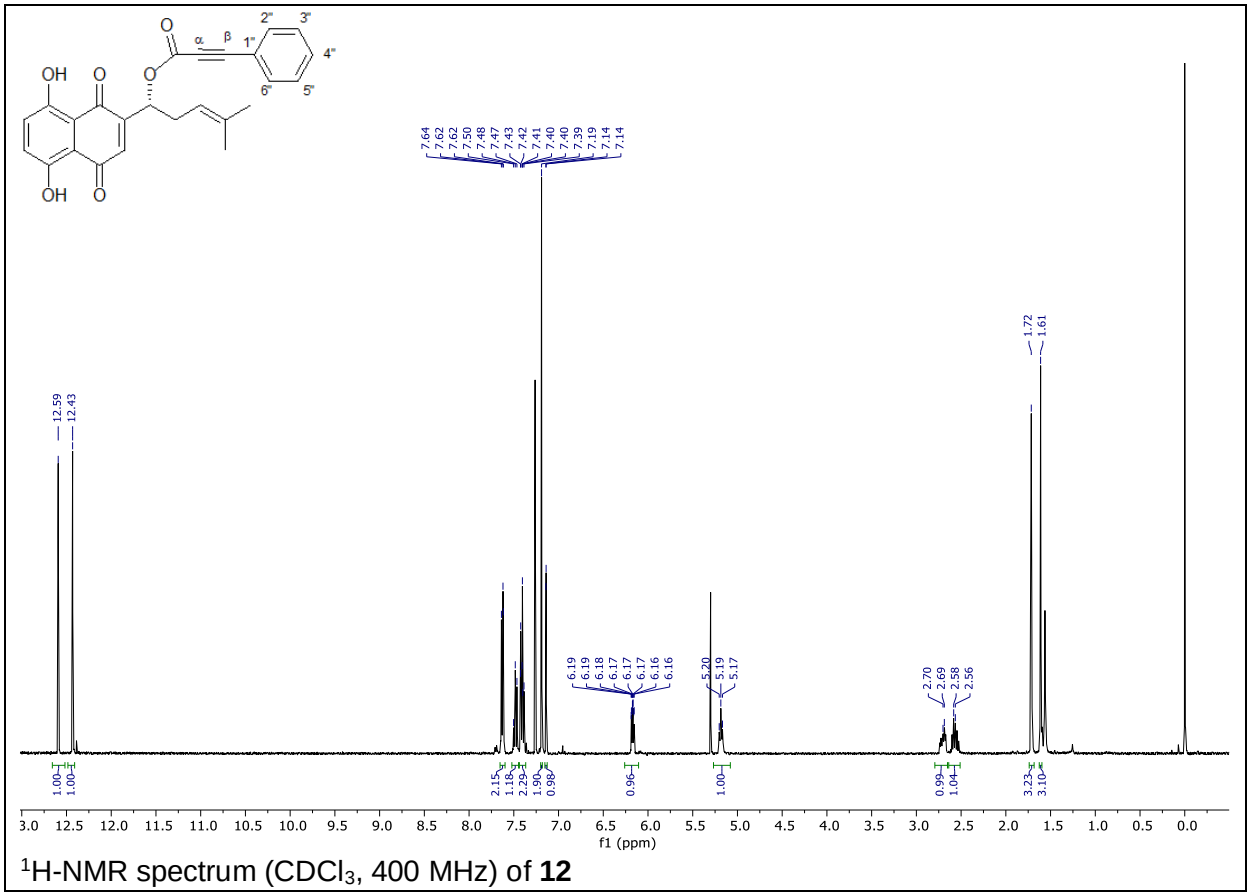
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **10**



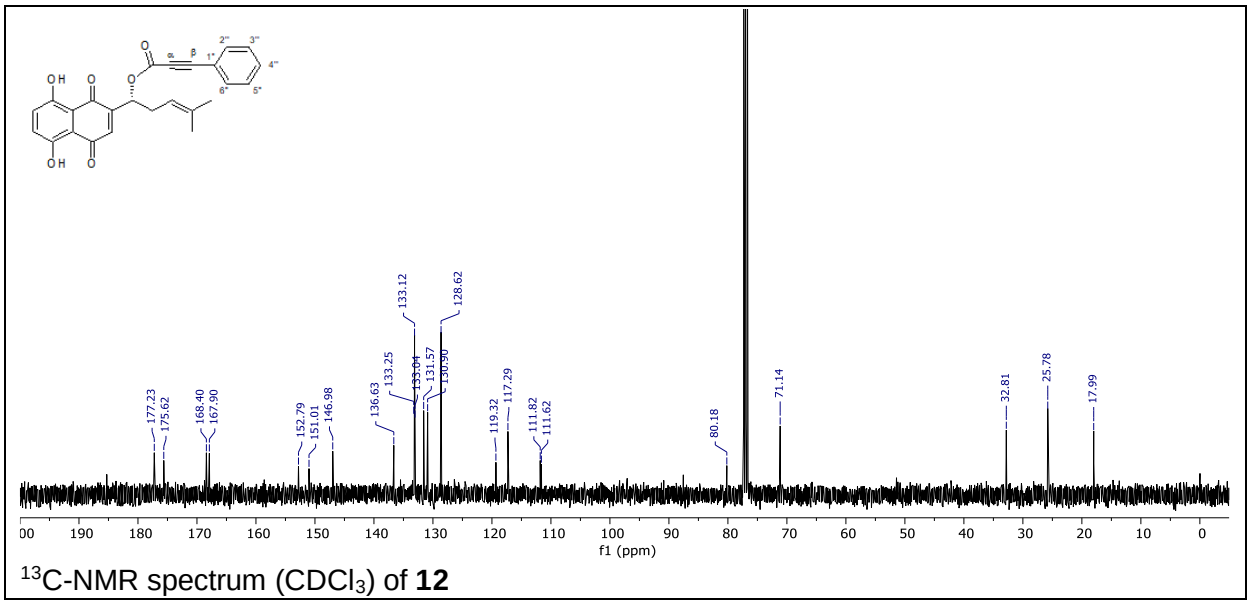
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **11**



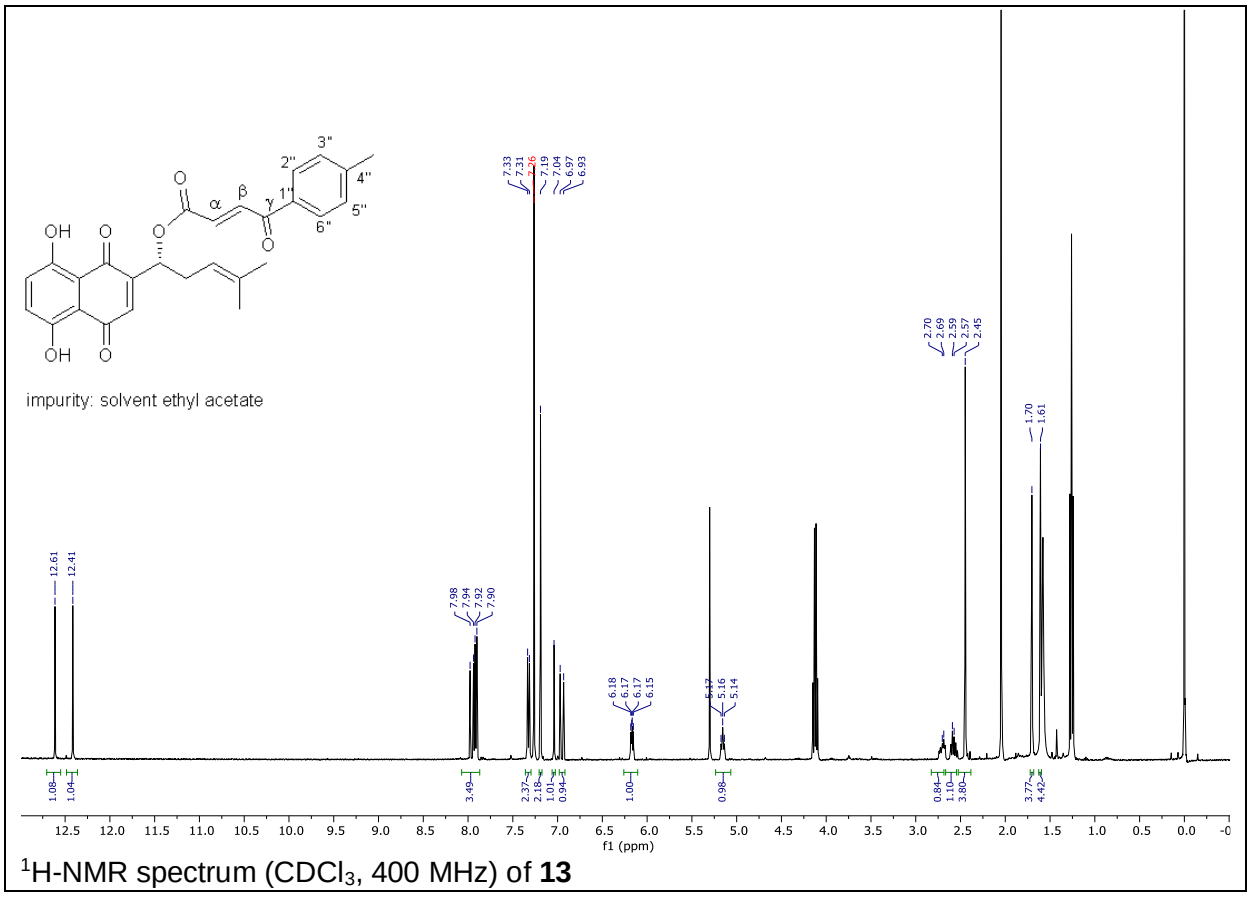
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **11**



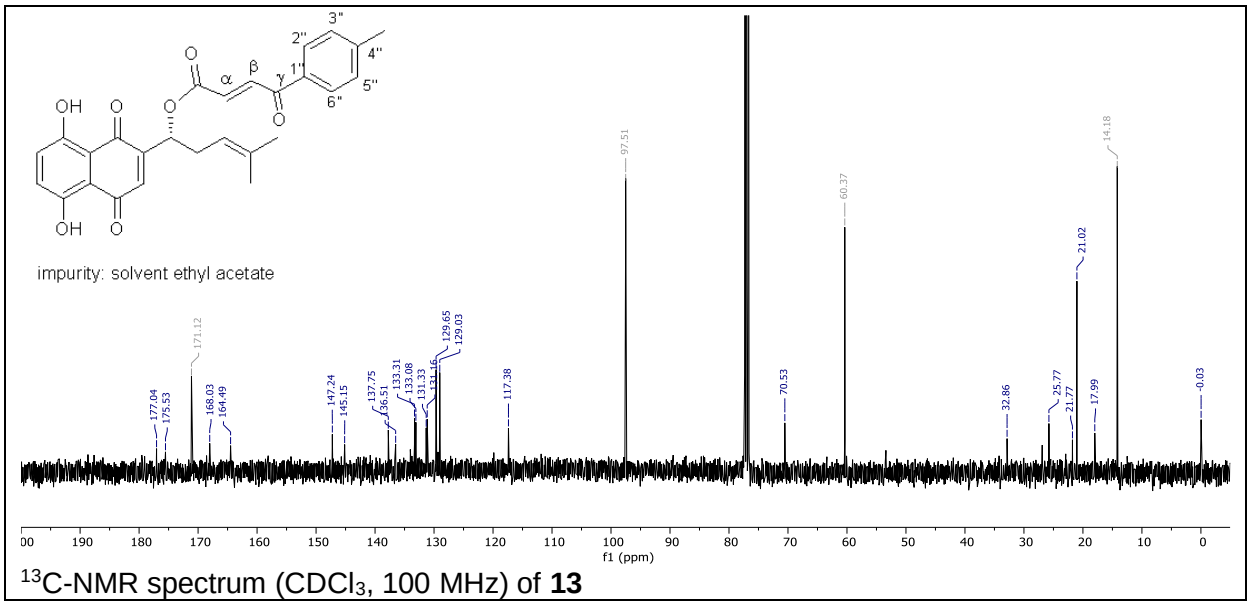
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **12**



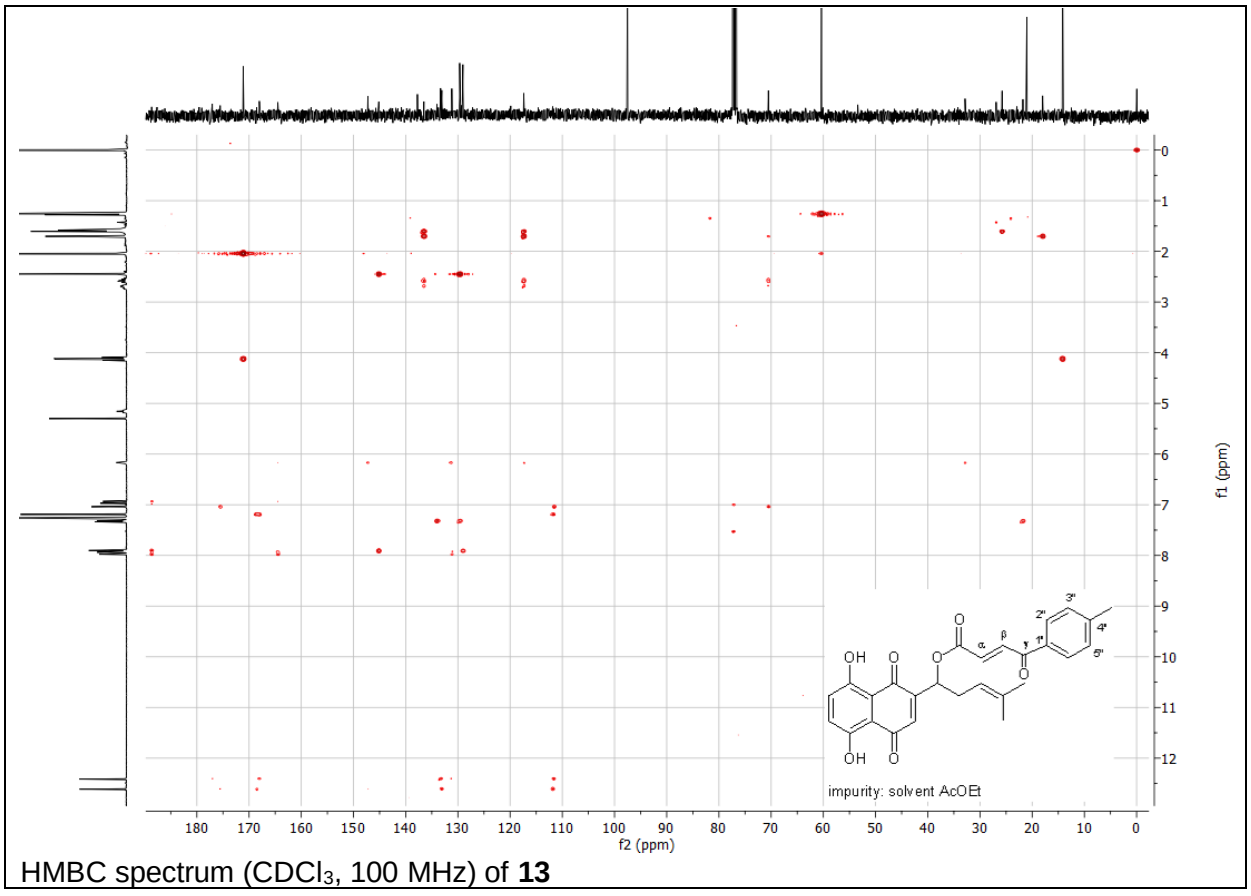
^{13}C-NMR spectrum ($CDCl_3$) of **12**



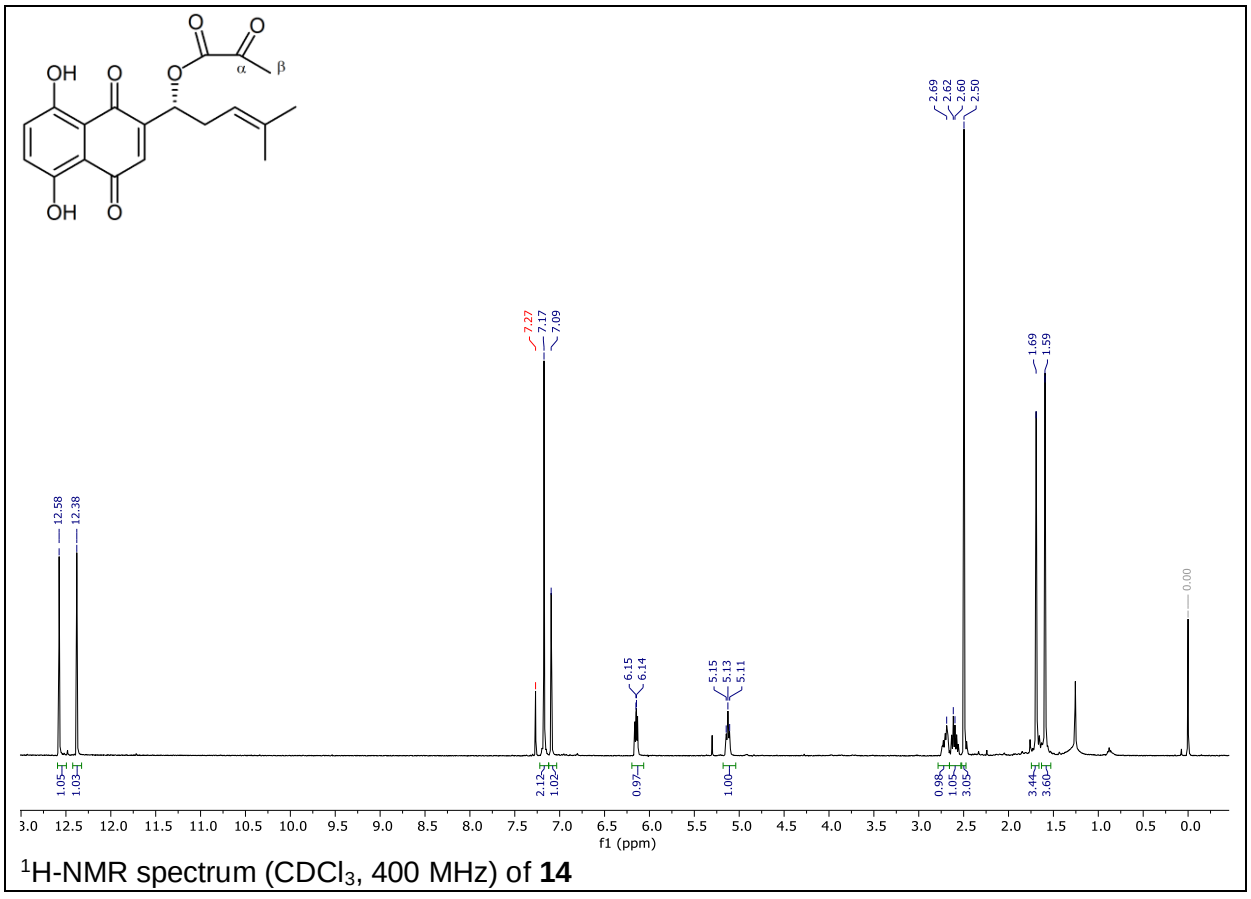
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **13**



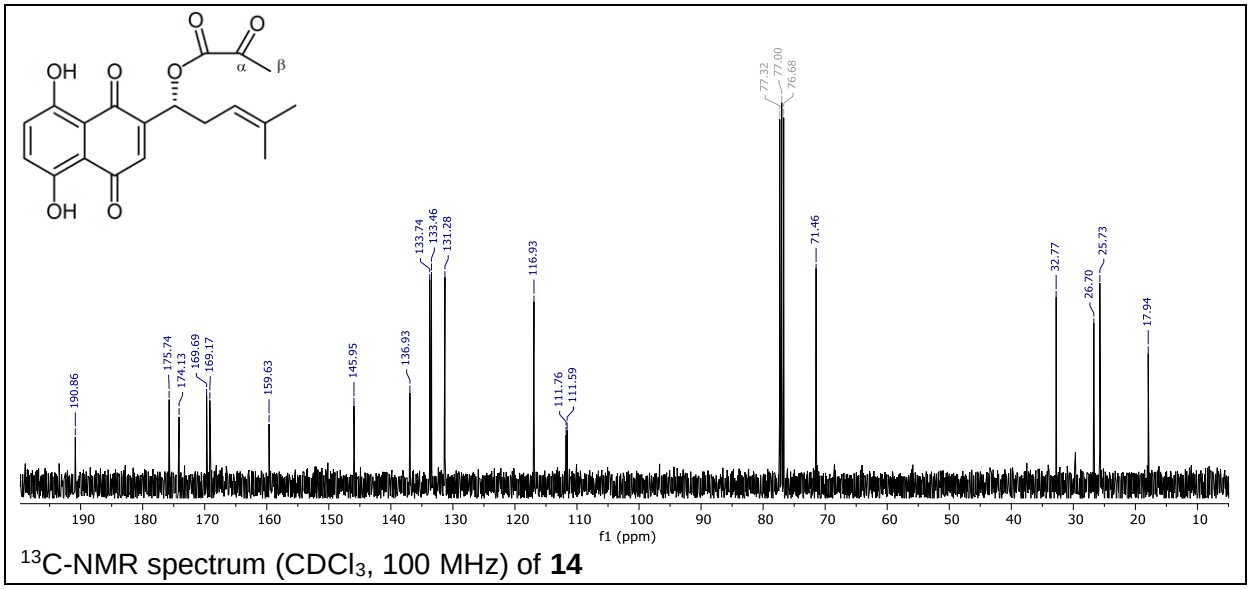
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **13**



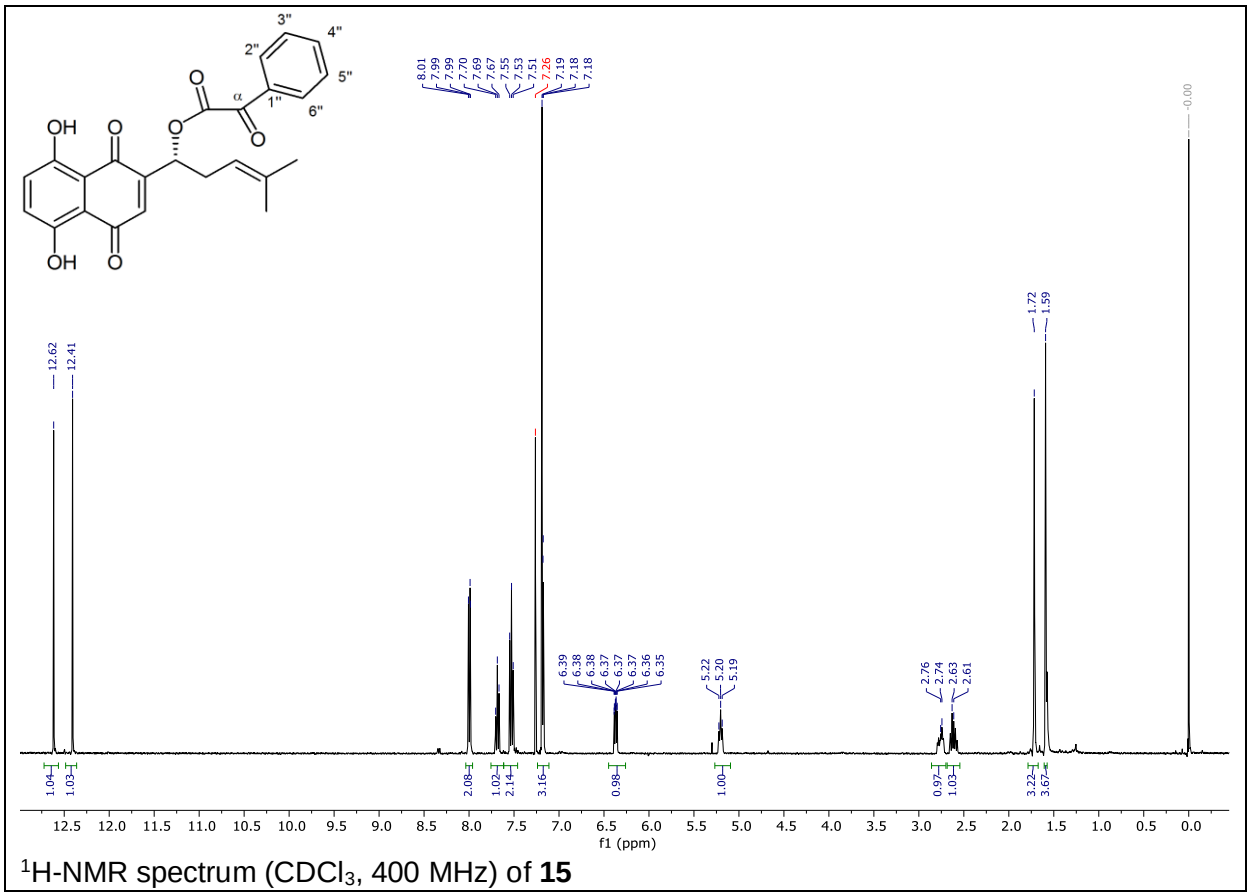
HMBC spectrum ($CDCl_3$, 100 MHz) of **13**



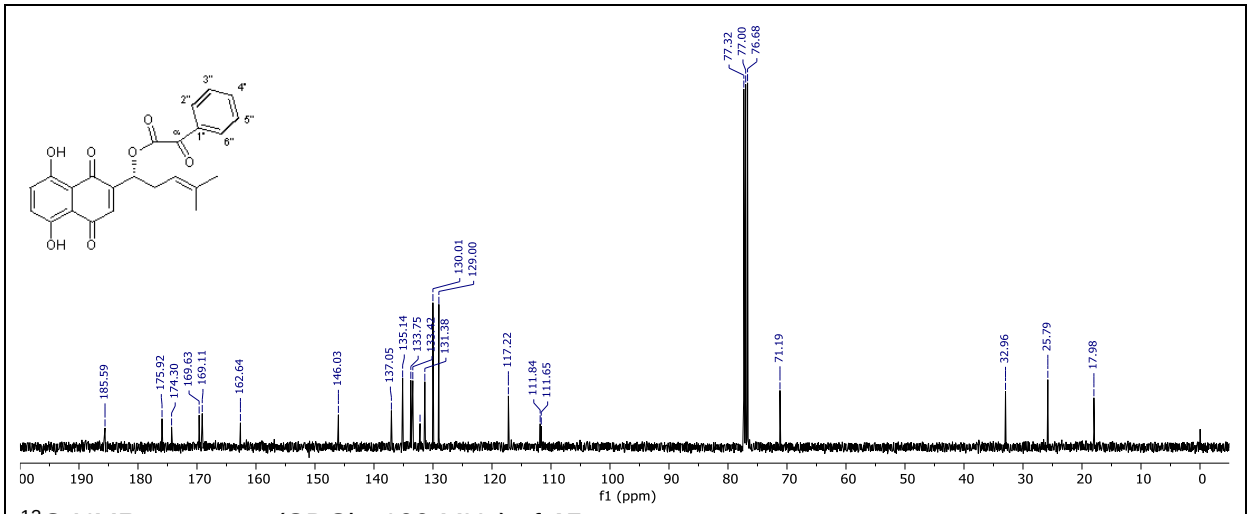
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **14**



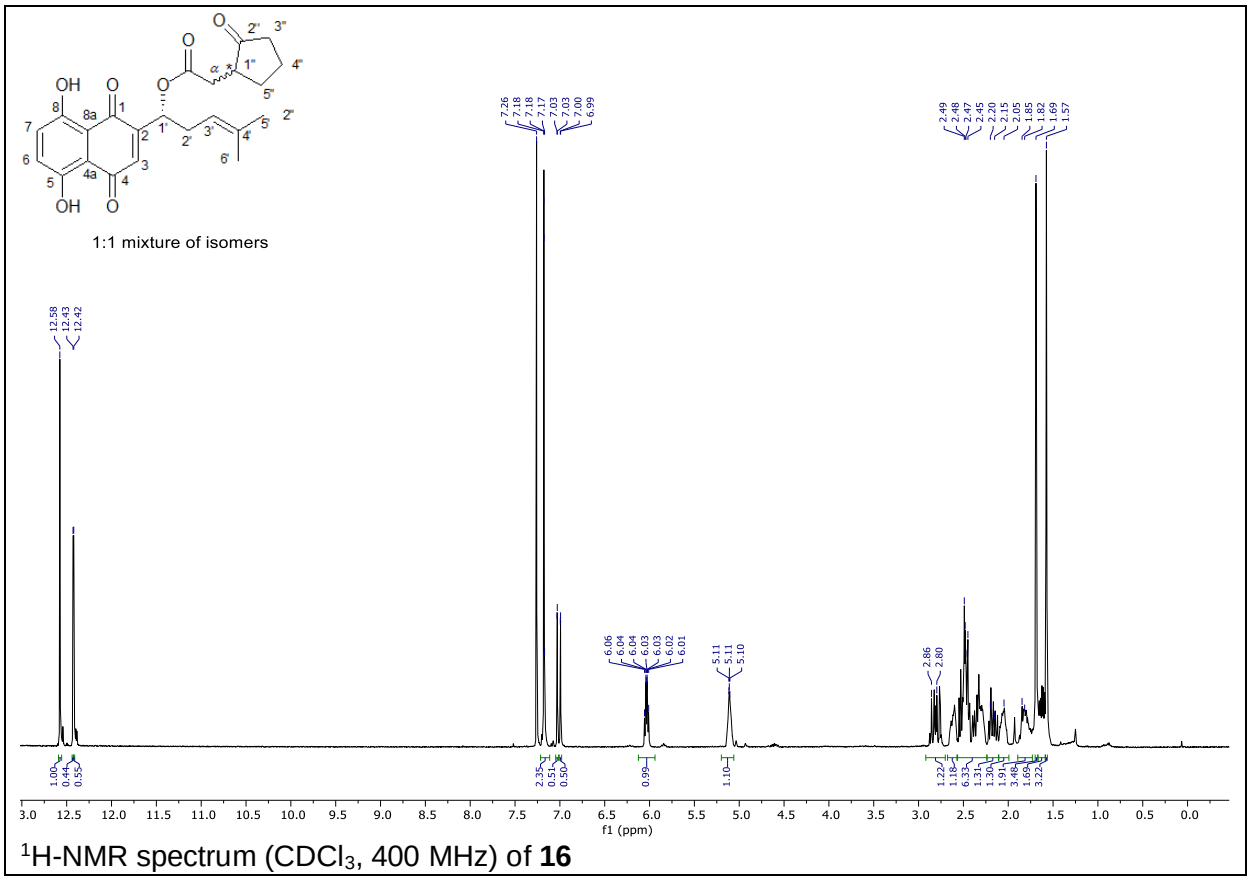
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **14**



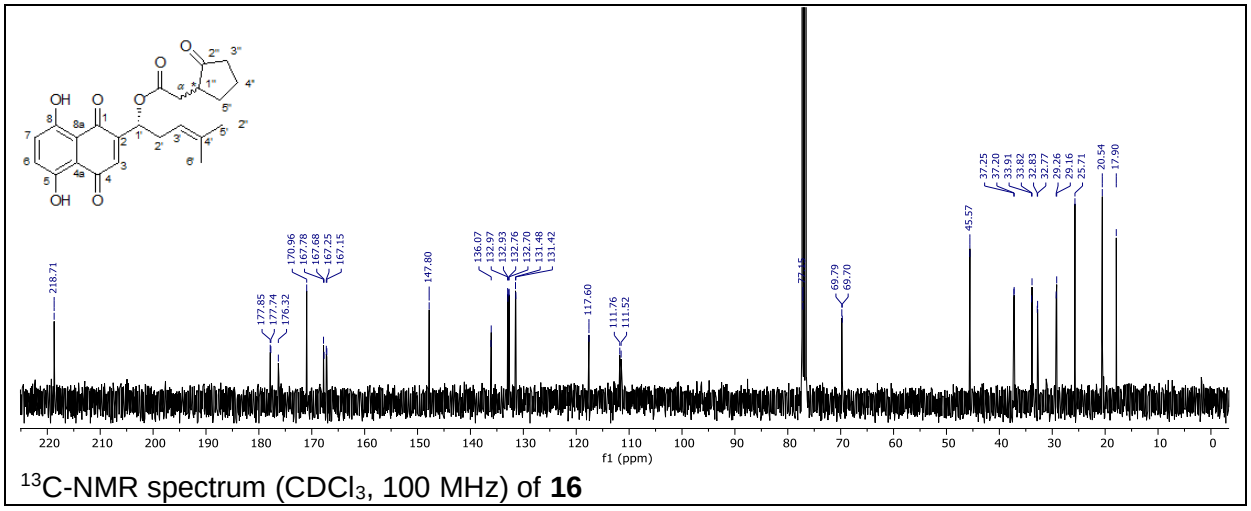
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **15**



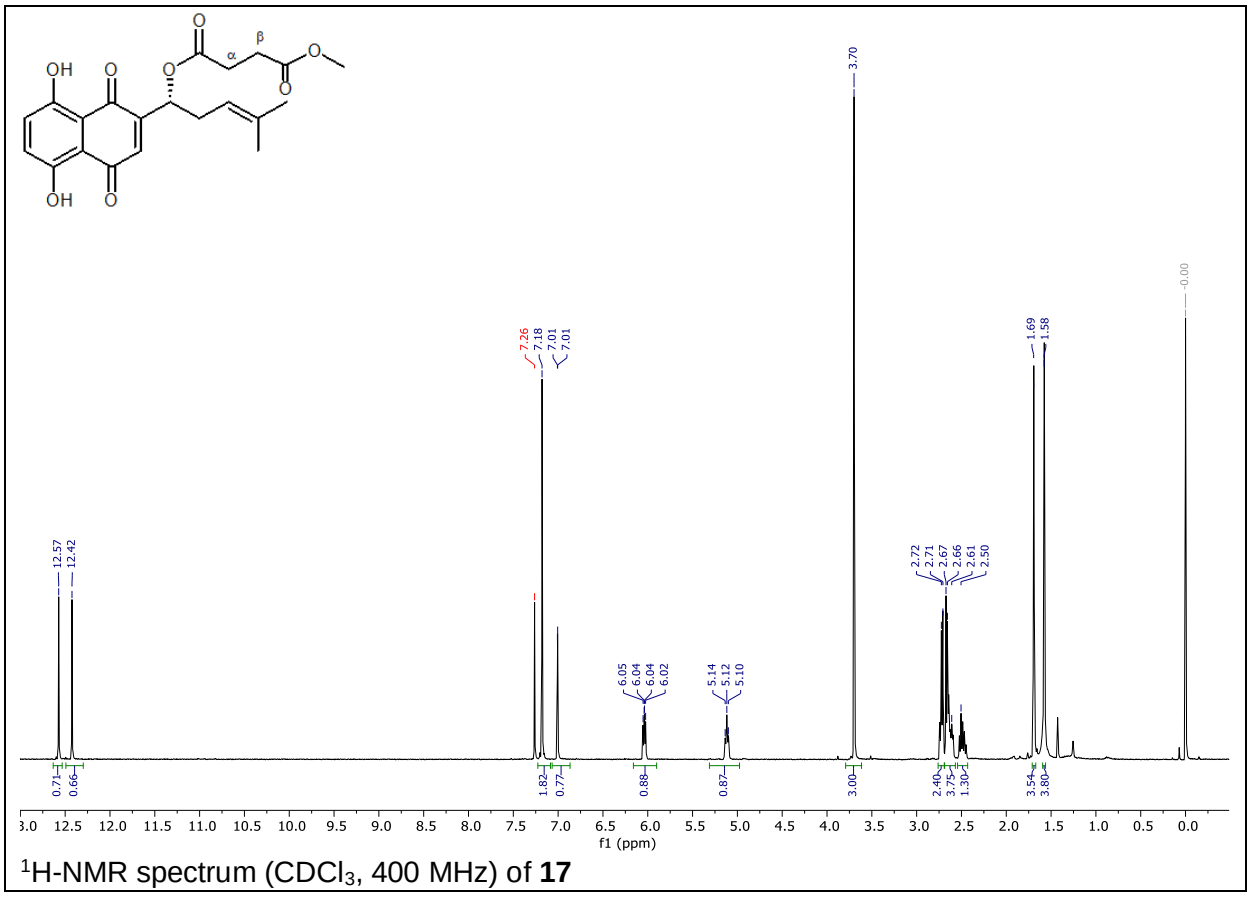
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **15**



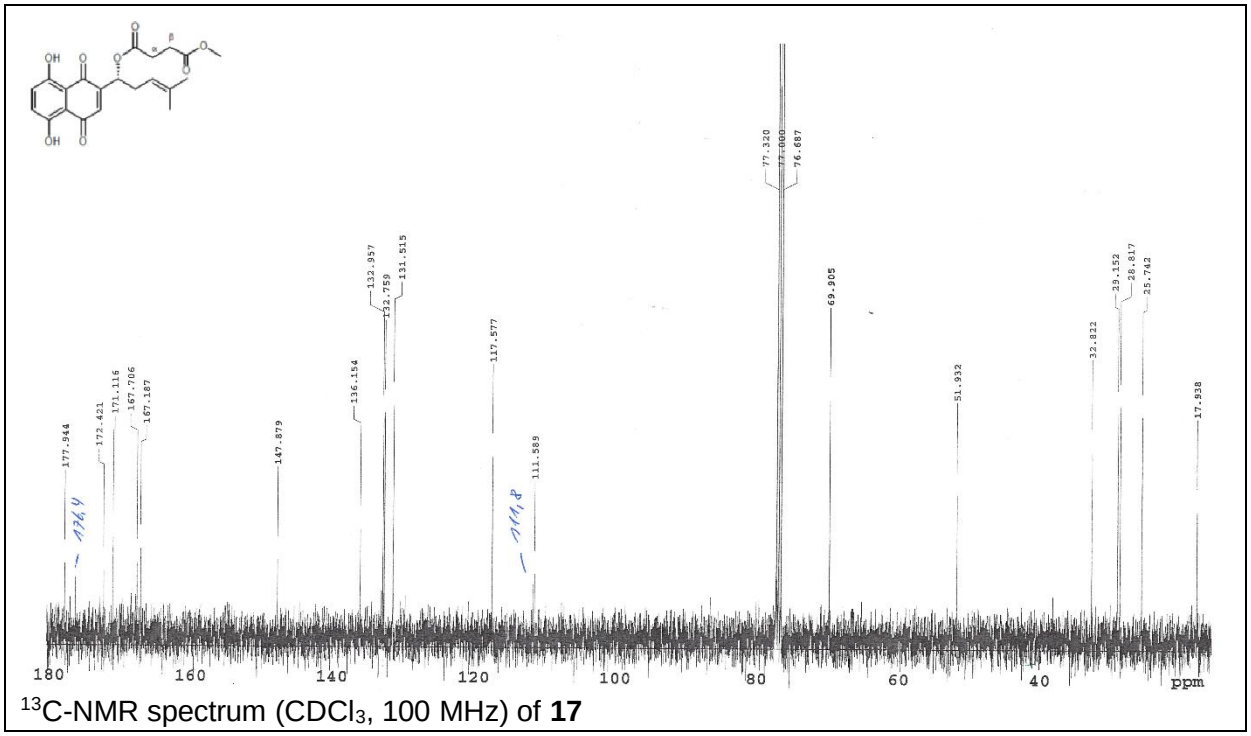
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **16**



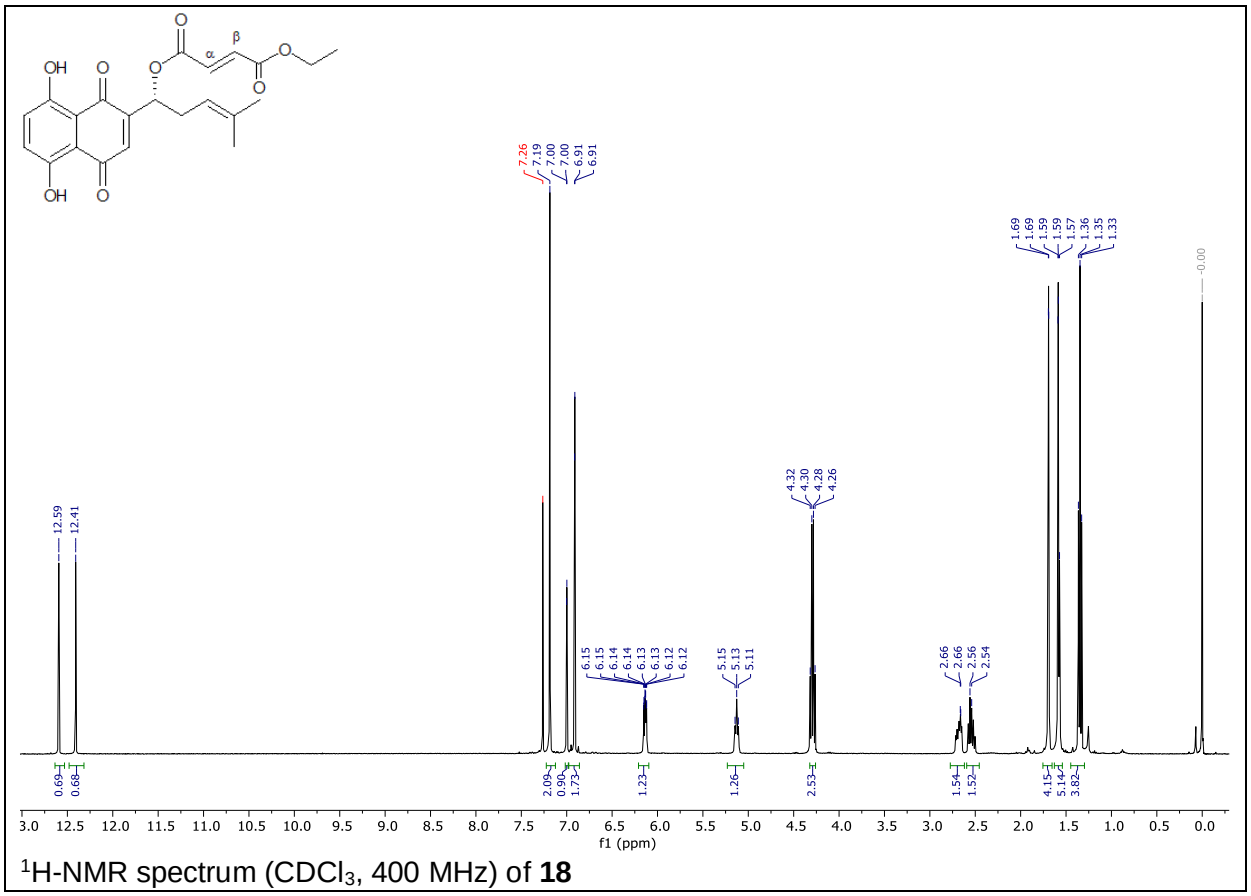
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **16**



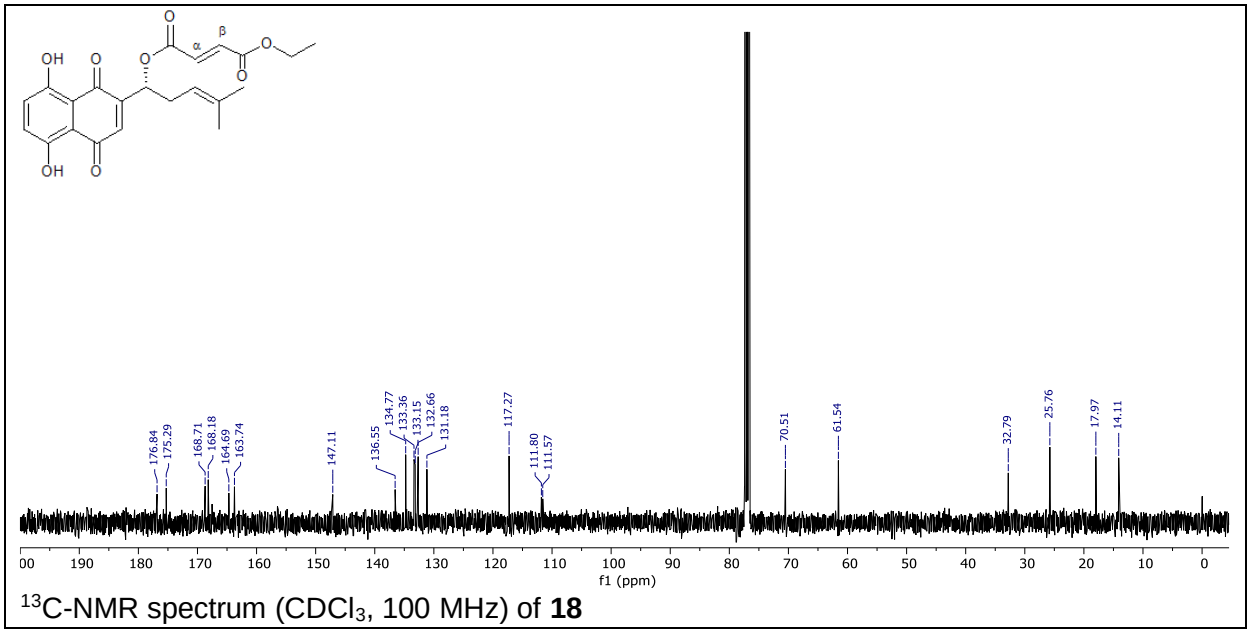
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **17**



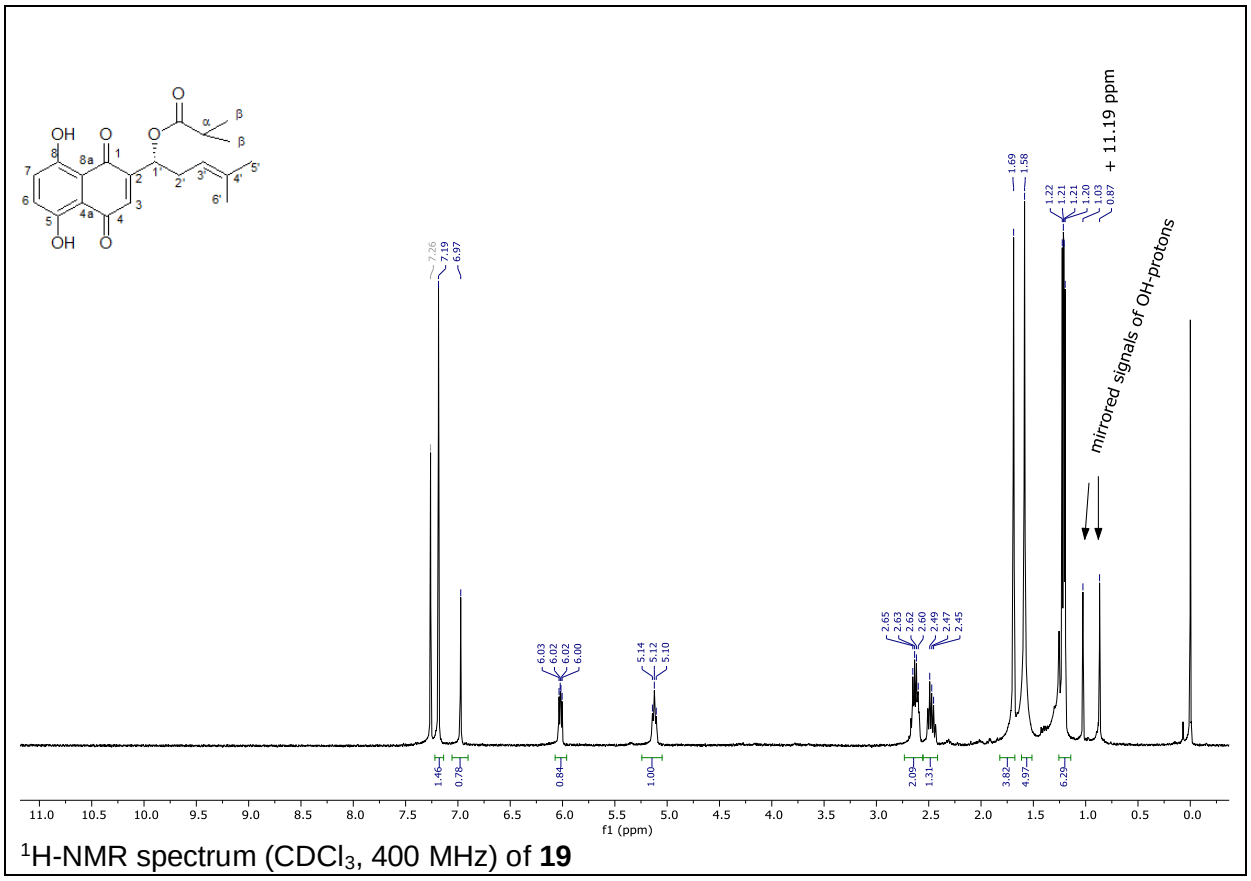
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **17**



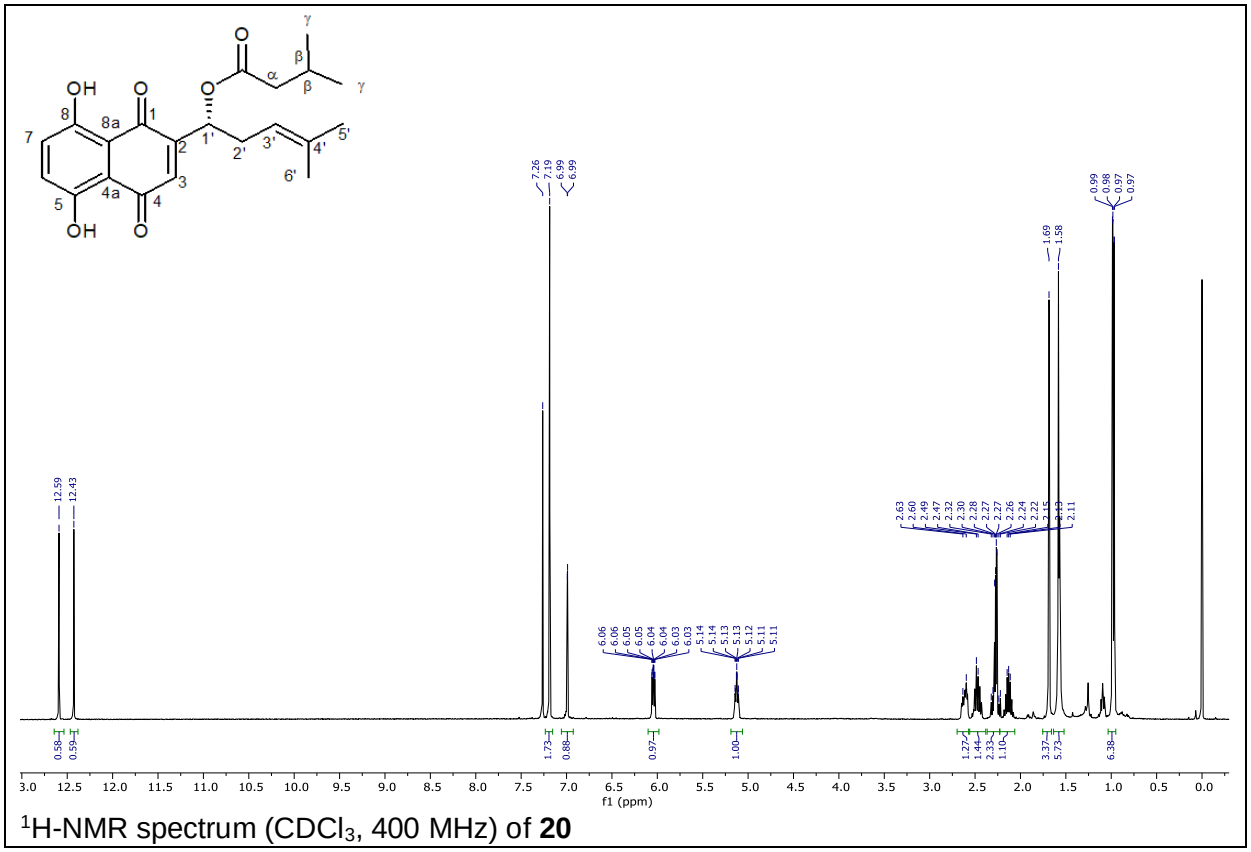
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **18**



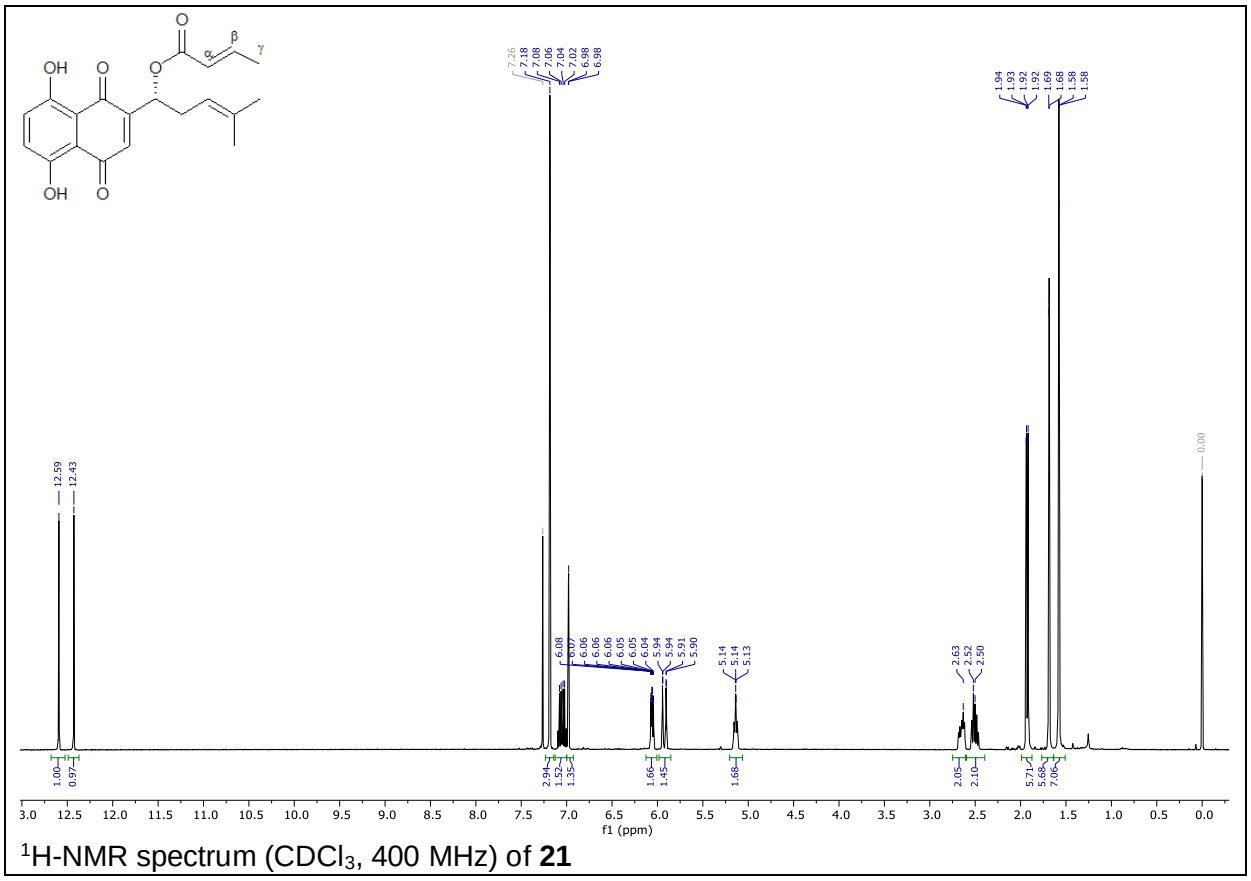
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **18**



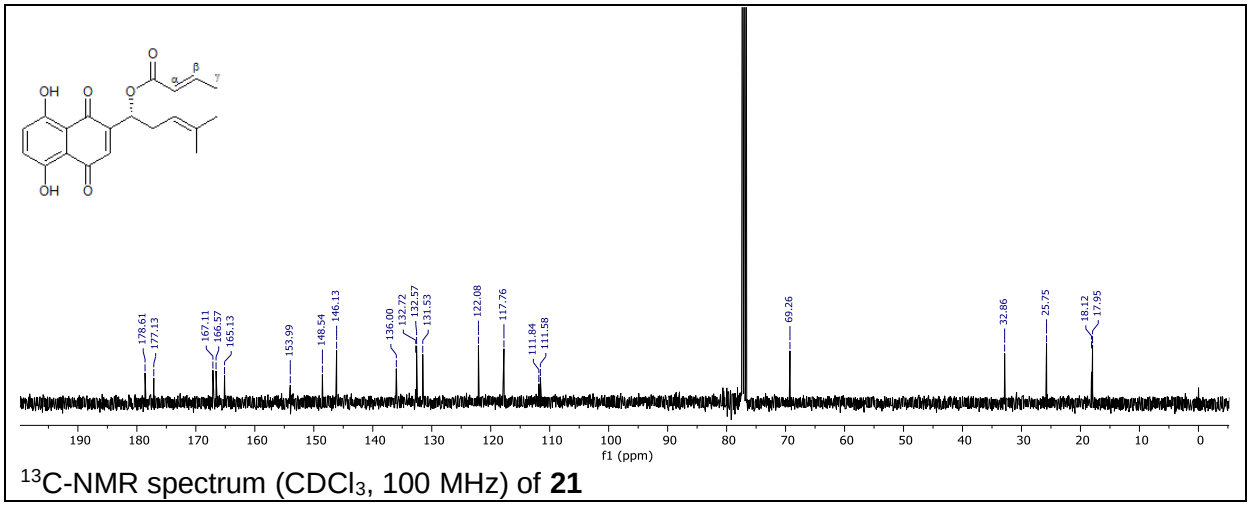
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **19**



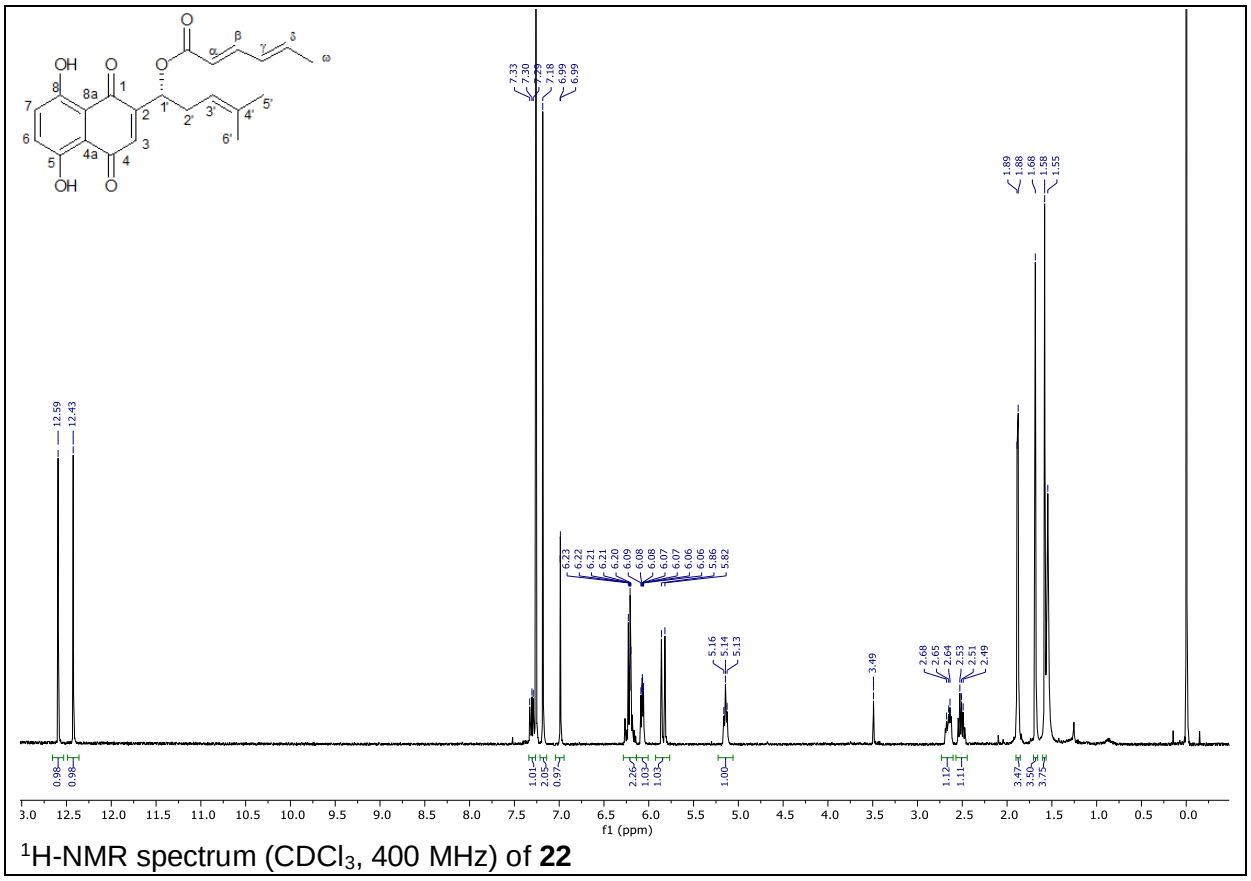
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **20**



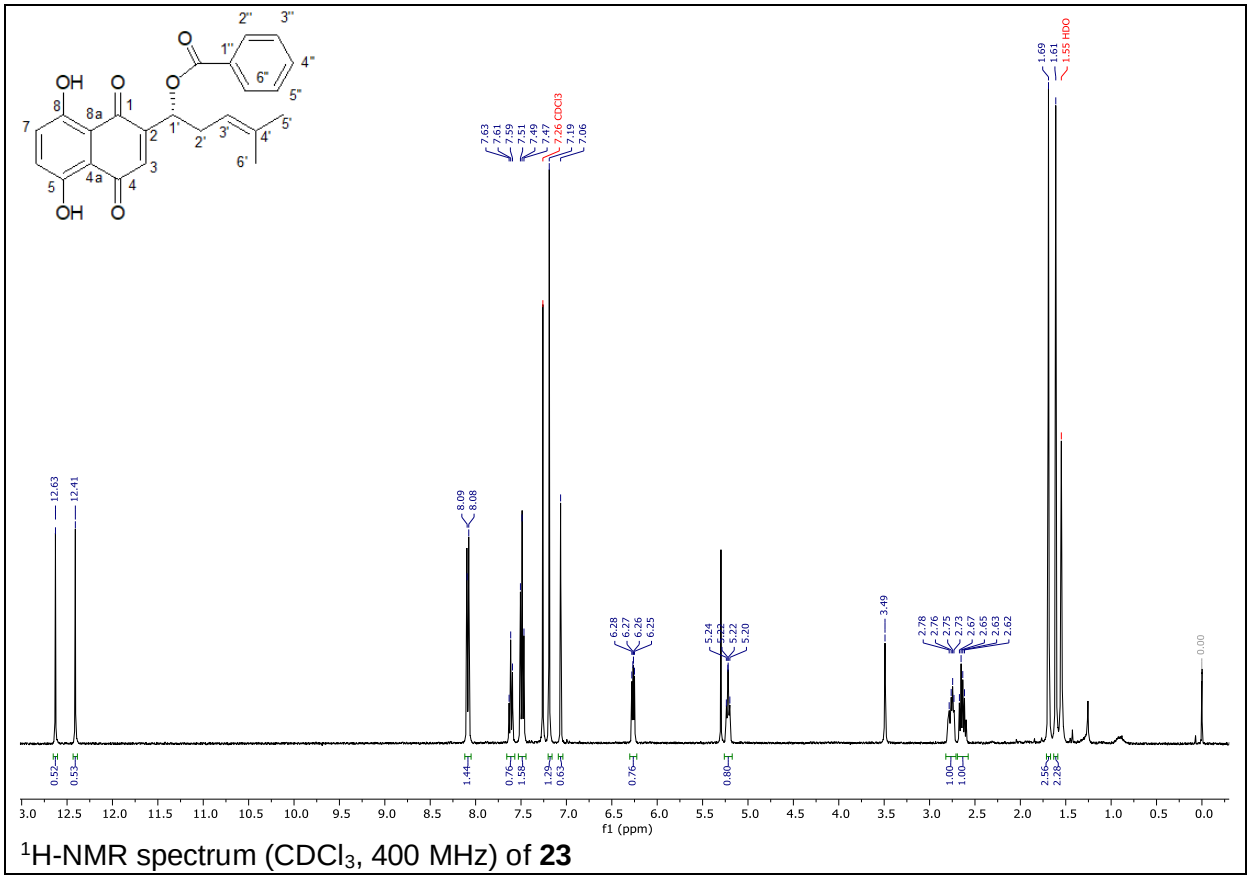
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **21**



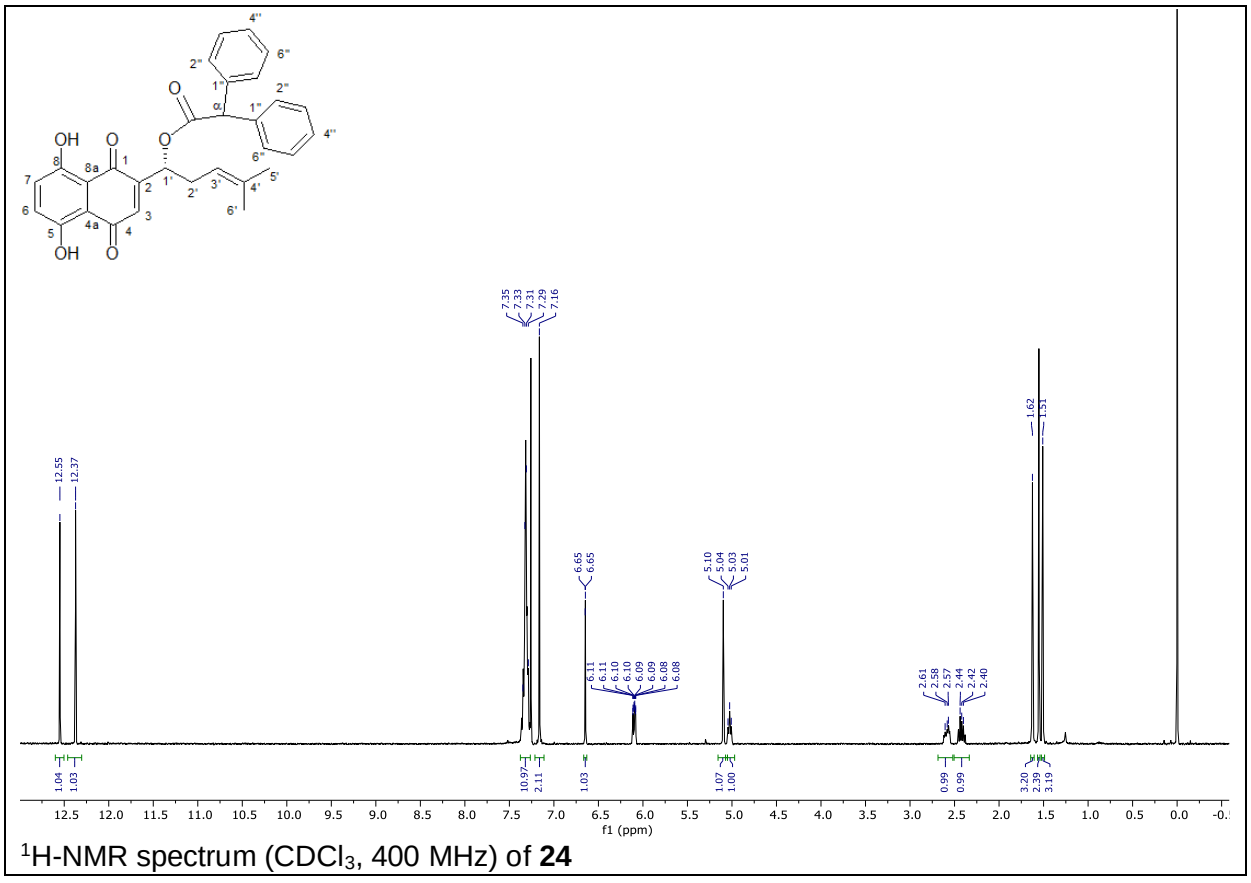
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **21**



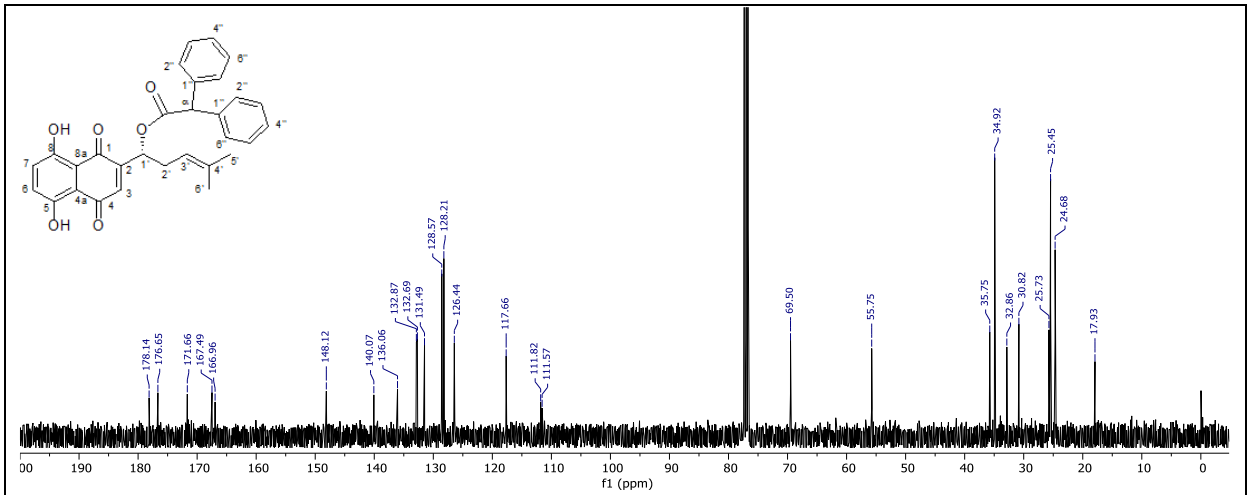
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **22**



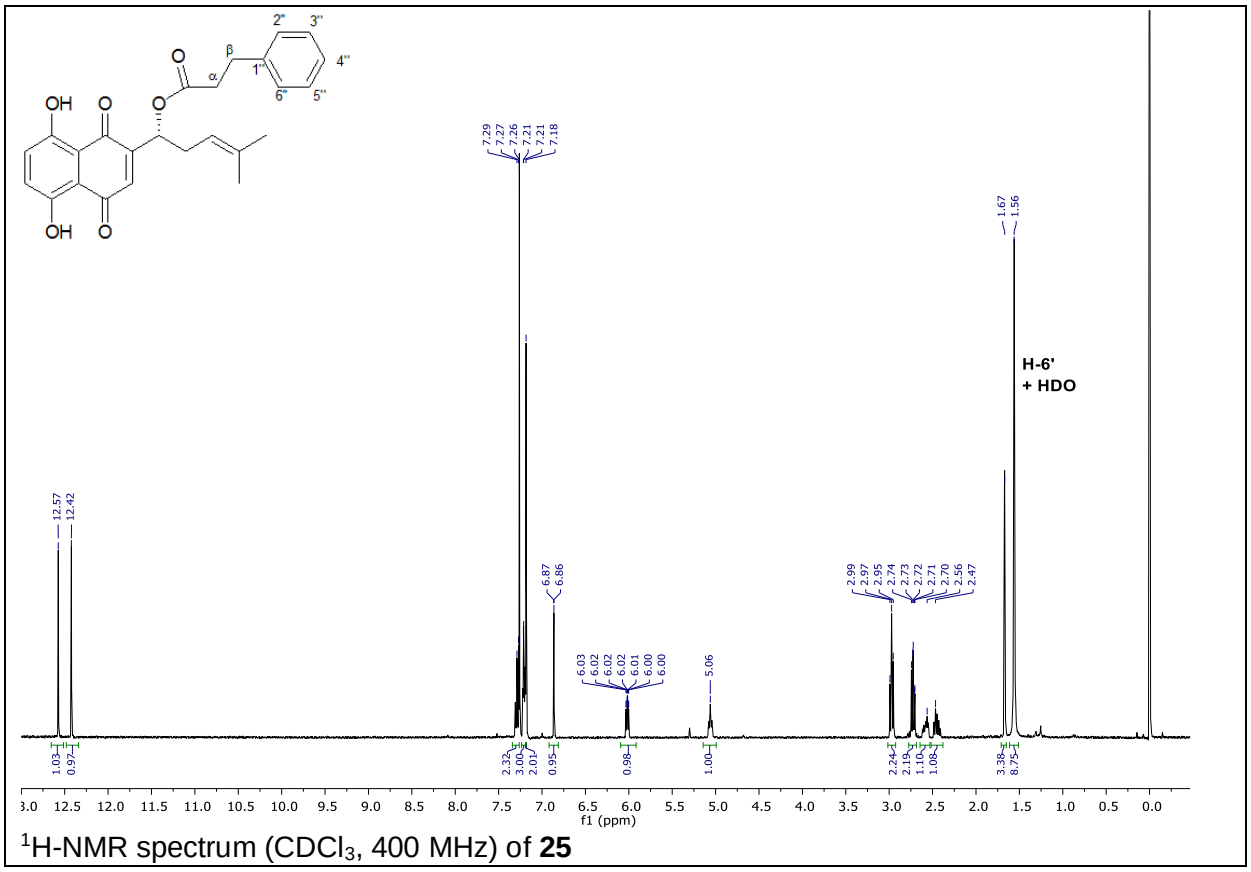
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **23**



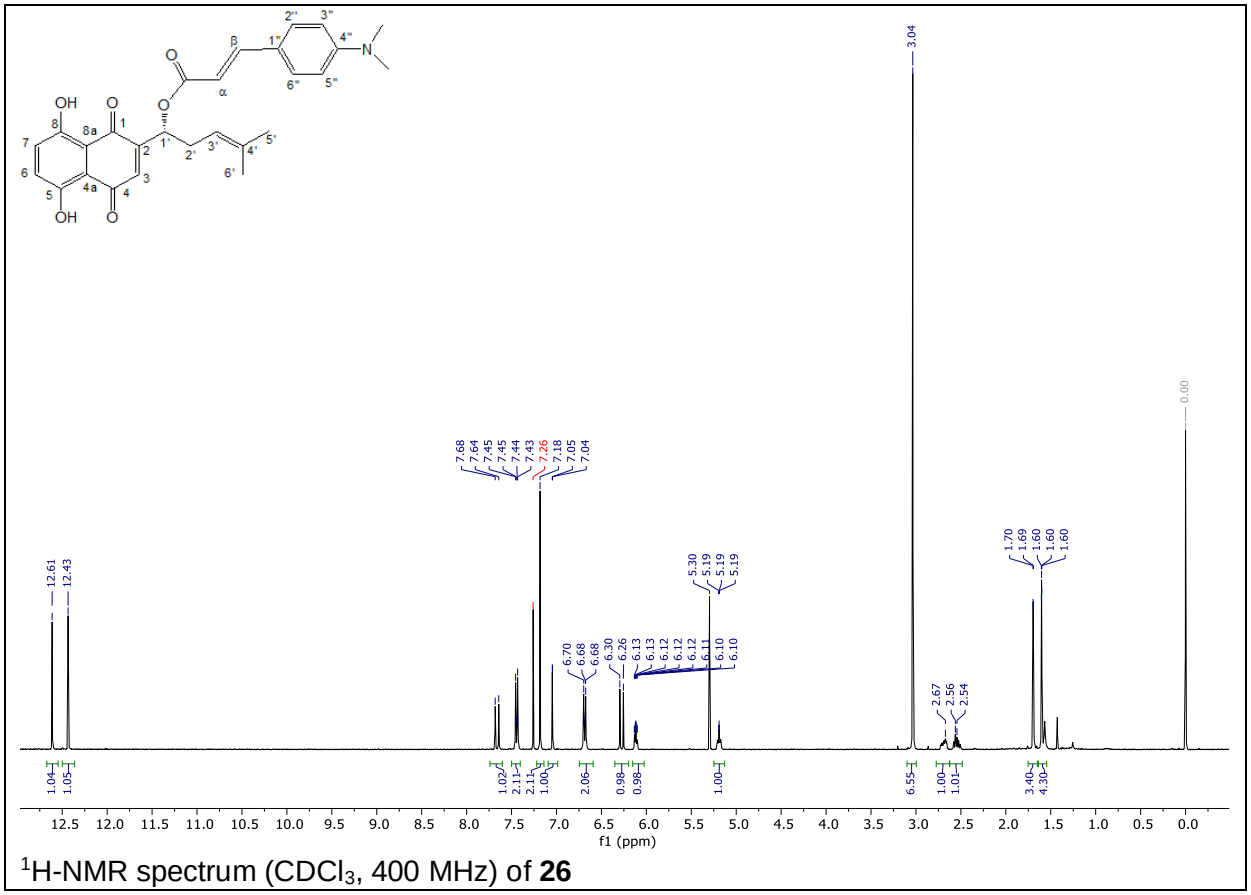
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **24**



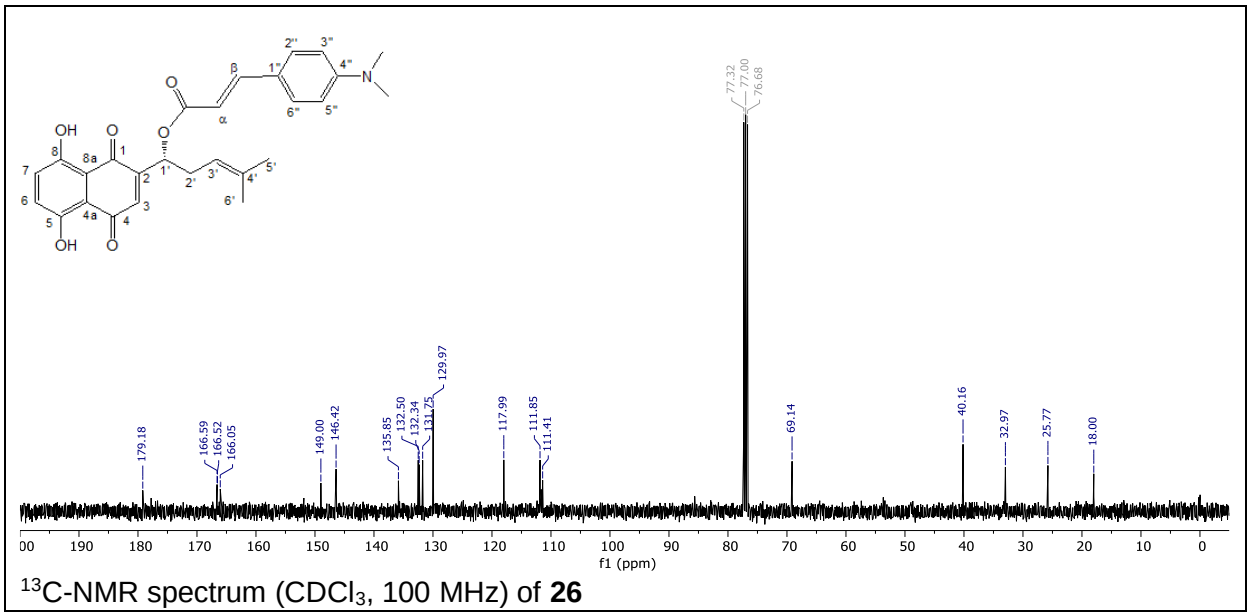
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **24**



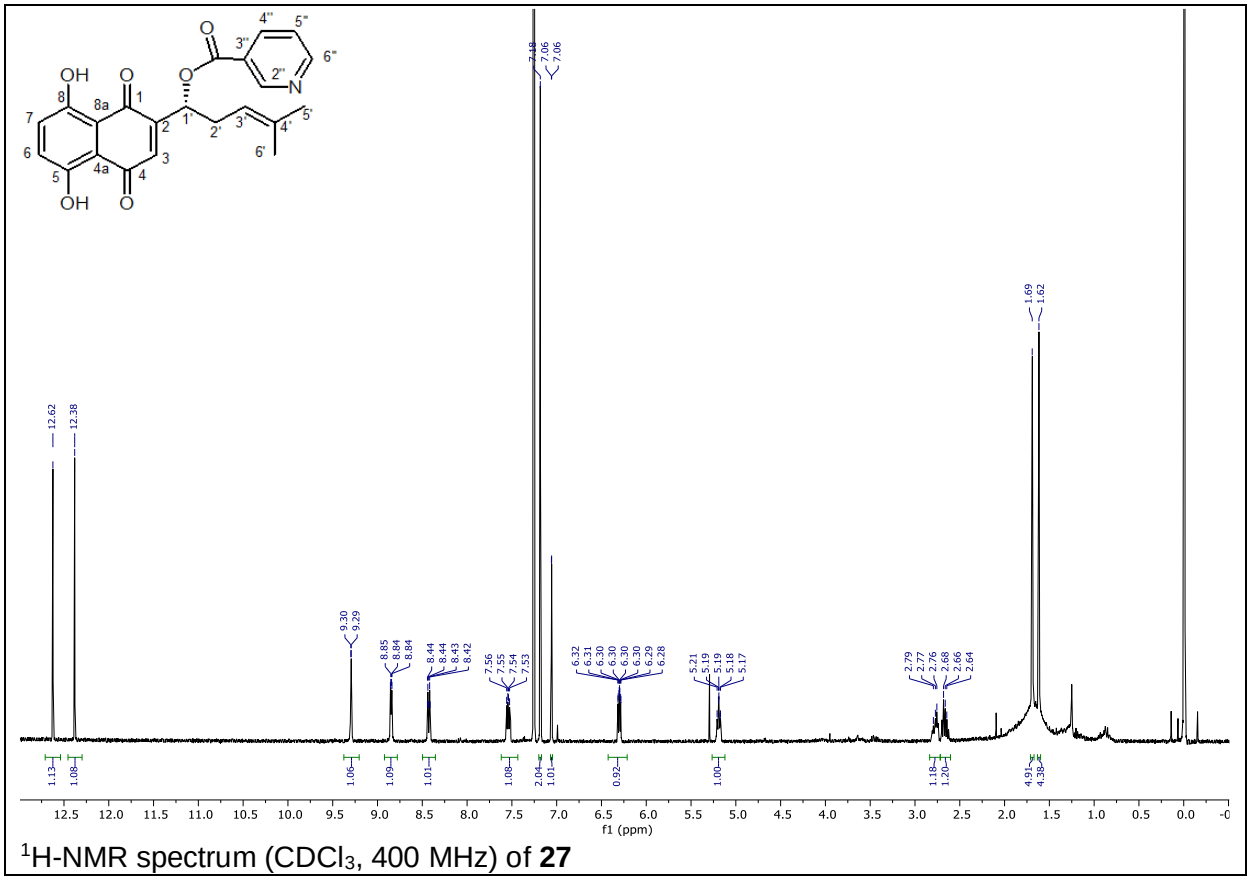
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **25**



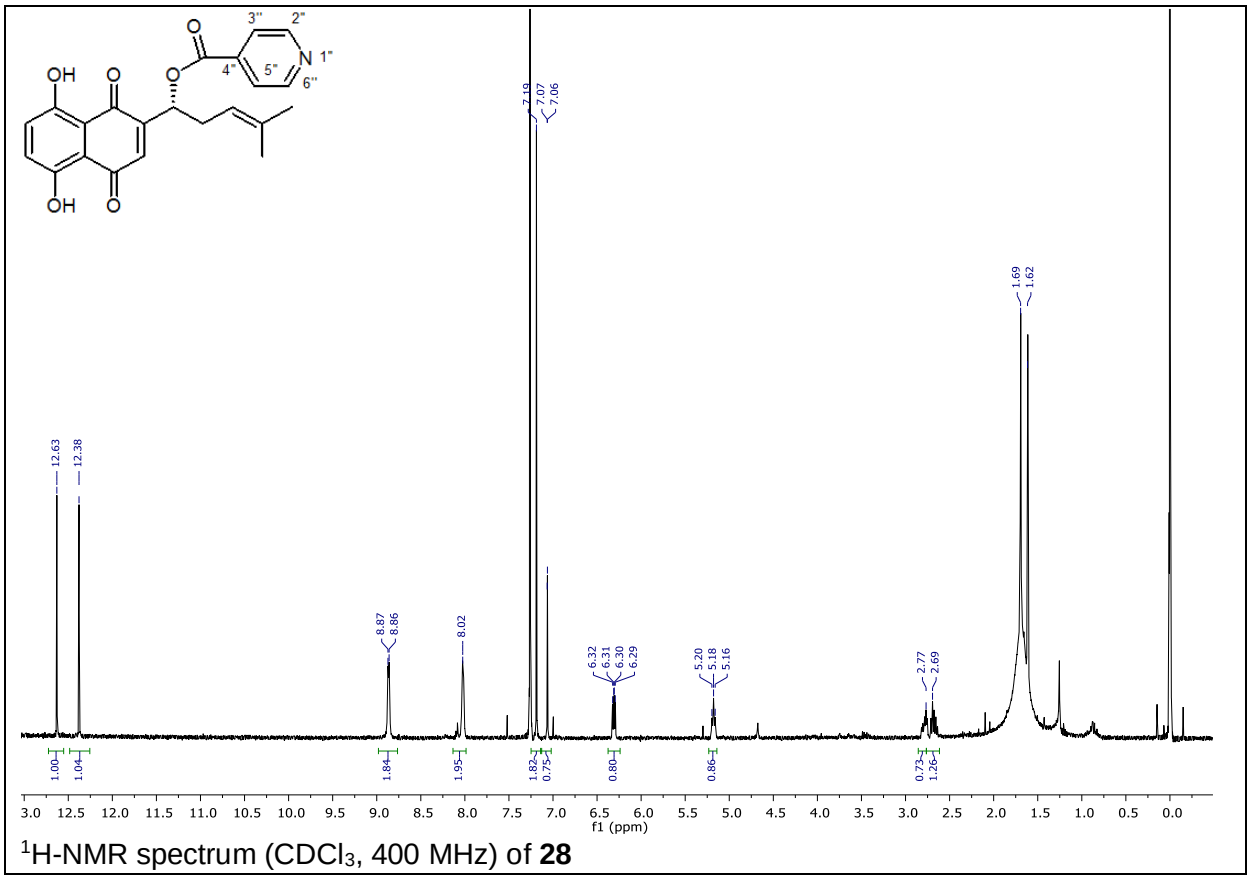
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **26**



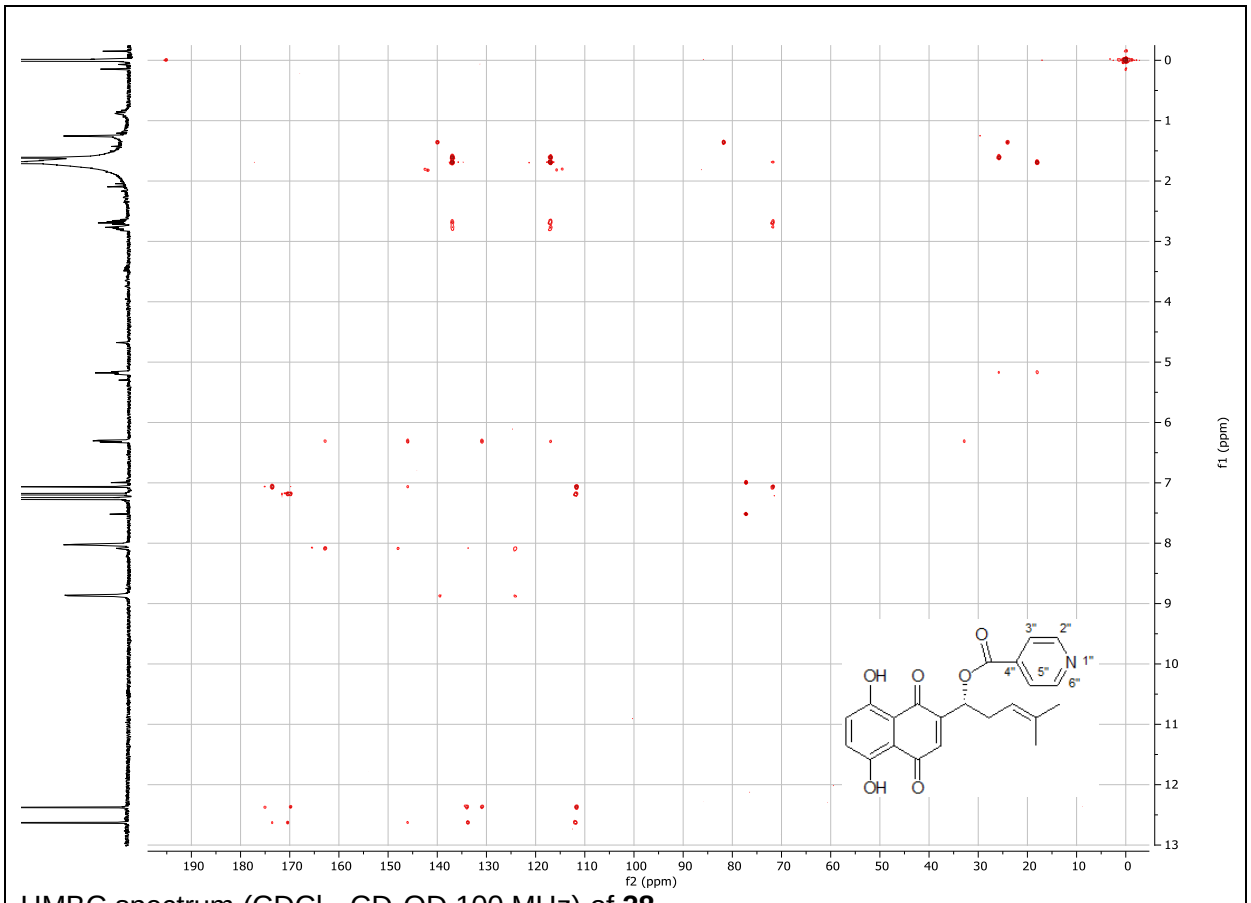
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **26**



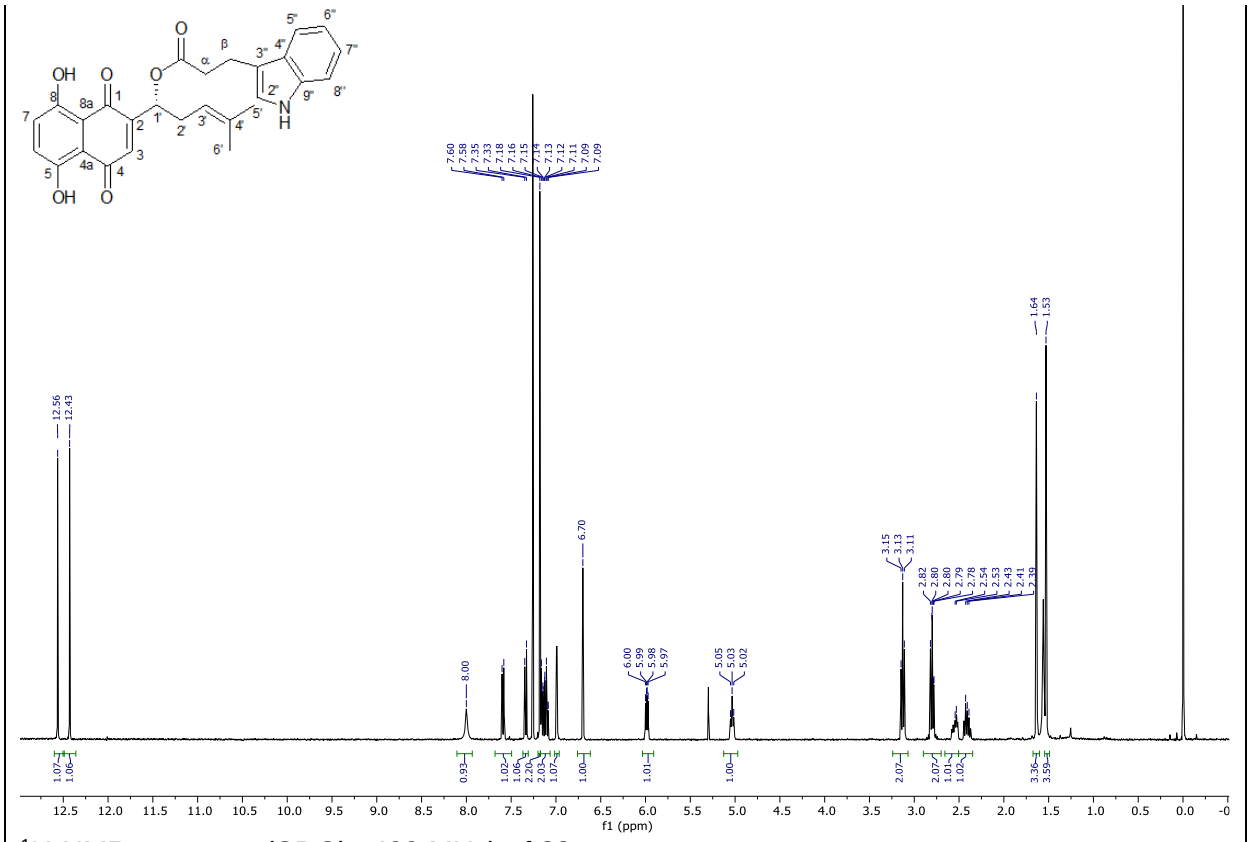
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **27**



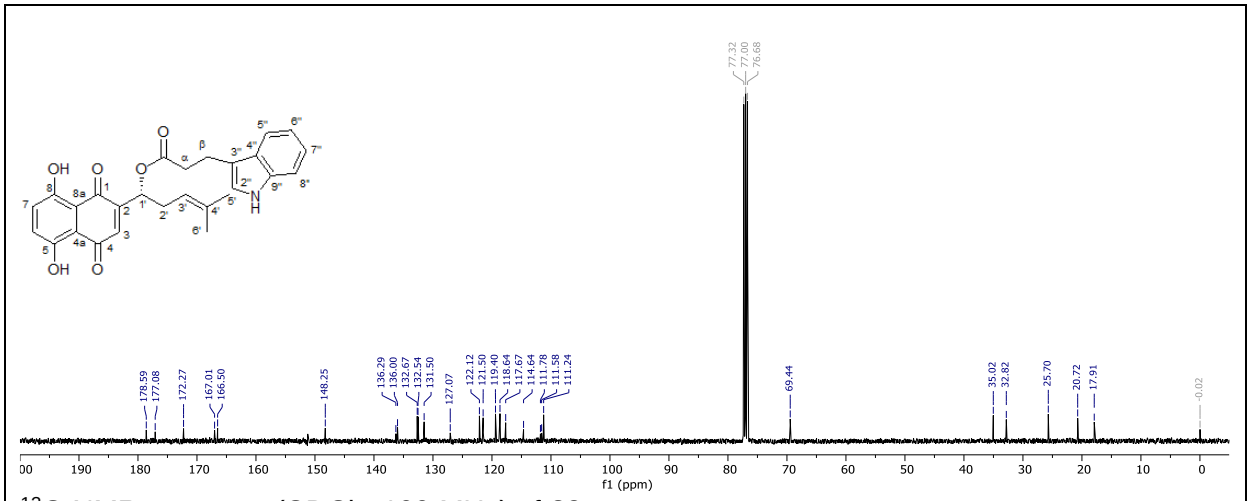
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **28**



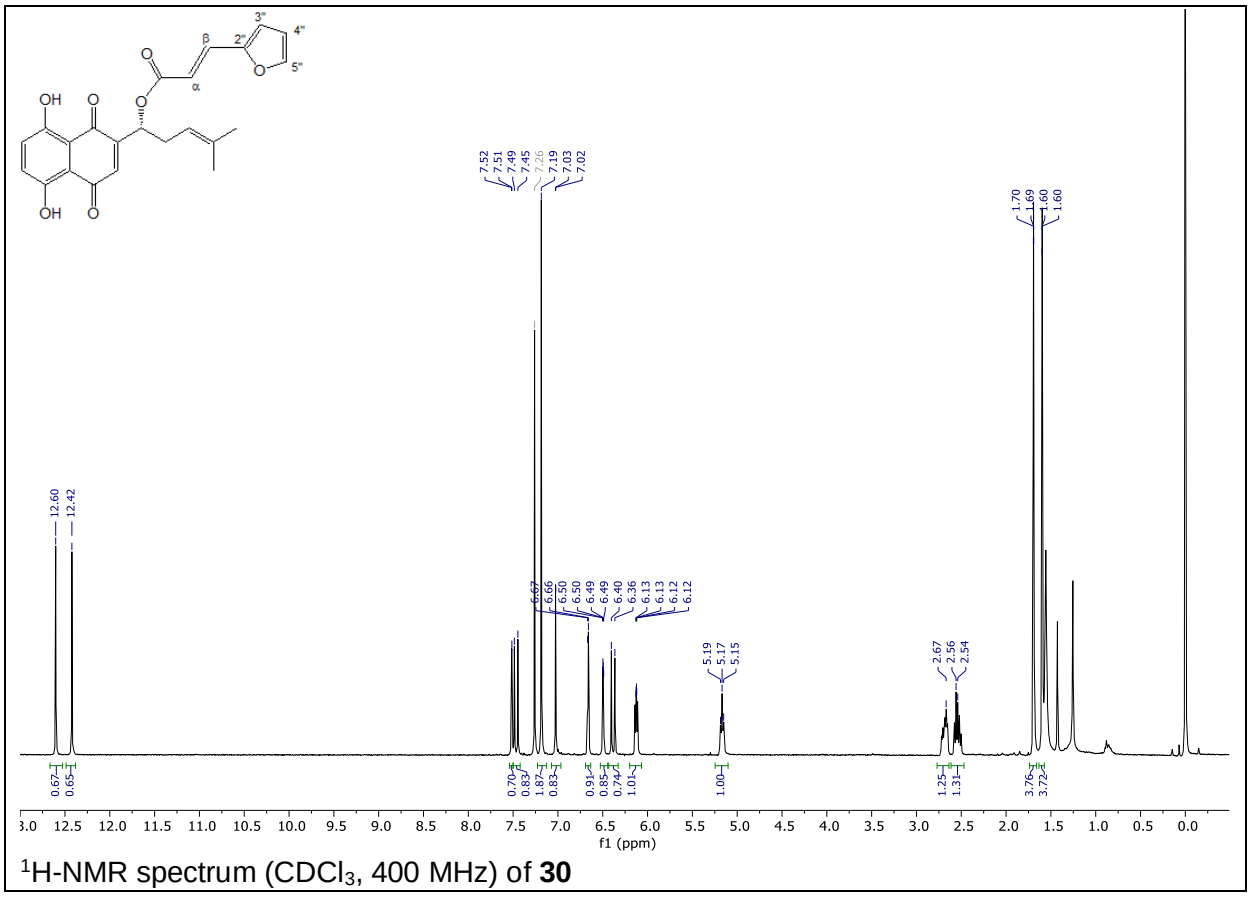
HMBC spectrum ($CDCl_3$, CD_3OD 100 MHz) of **28**



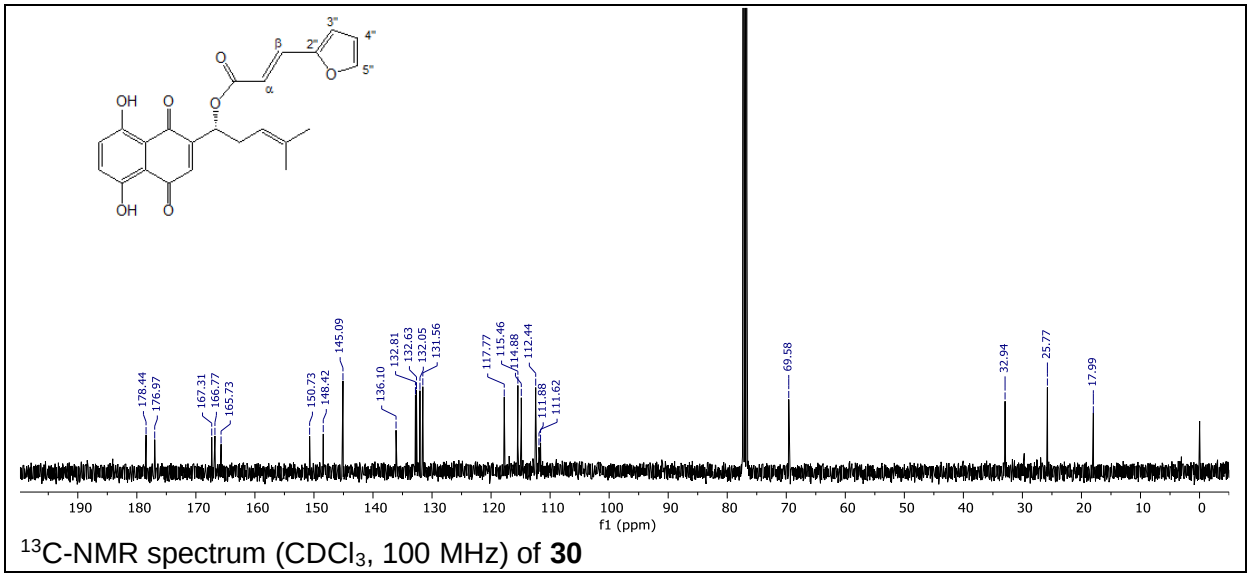
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **29**



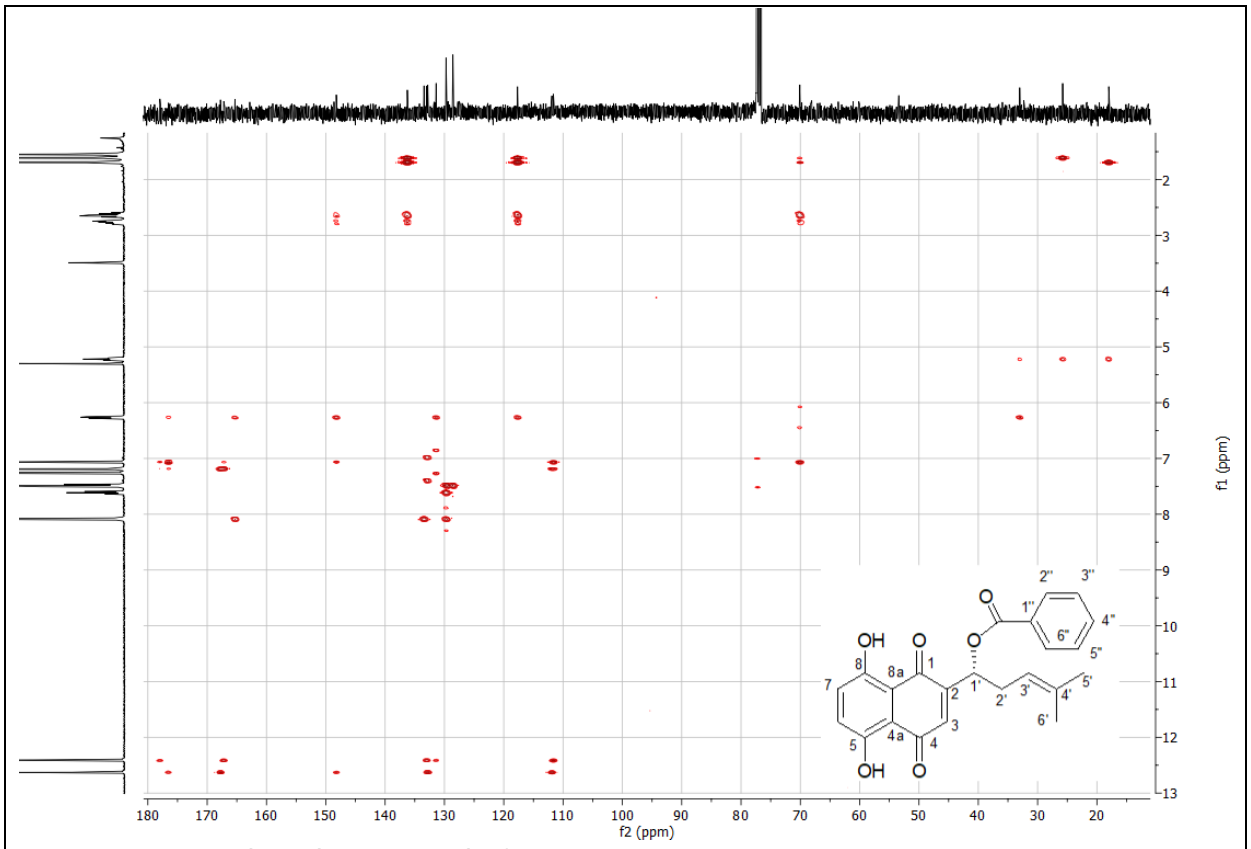
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **29**



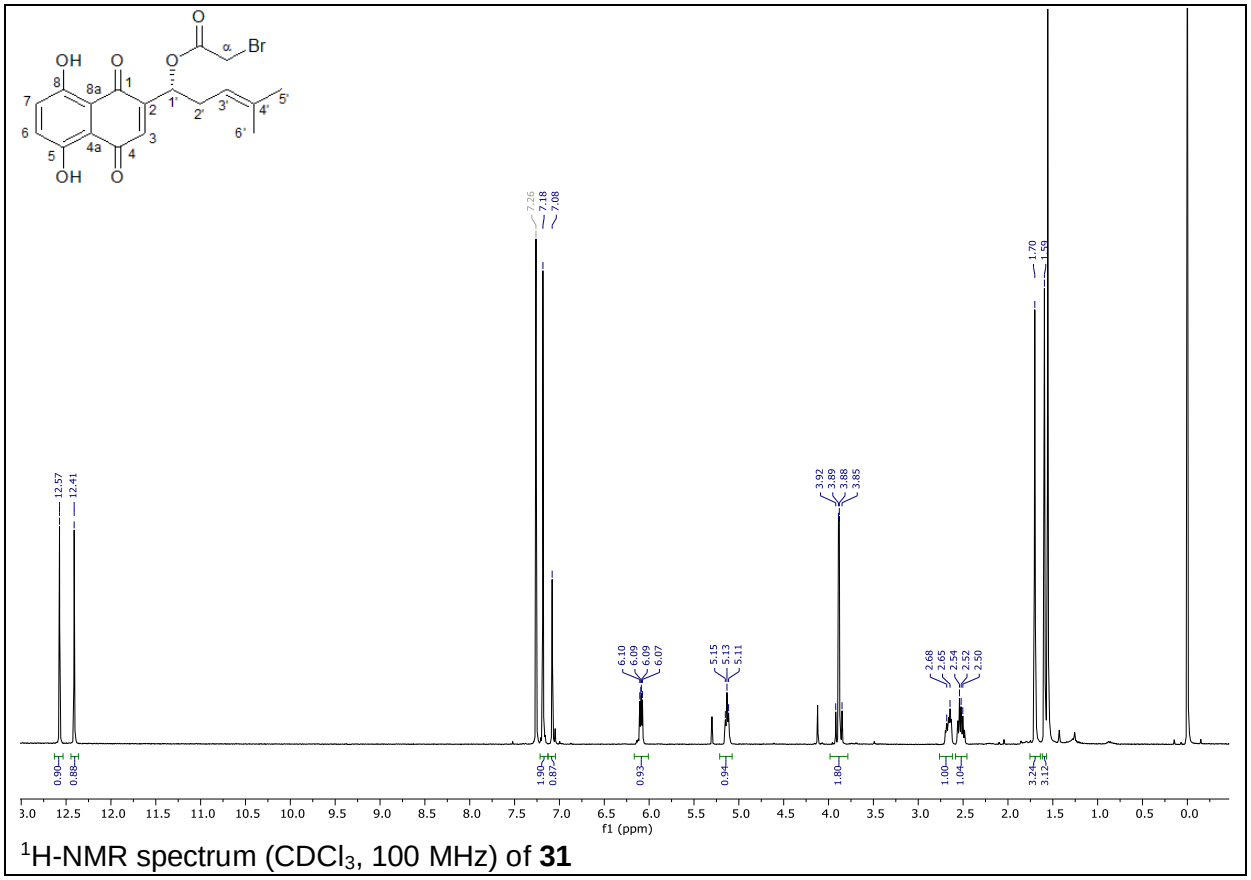
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **30**



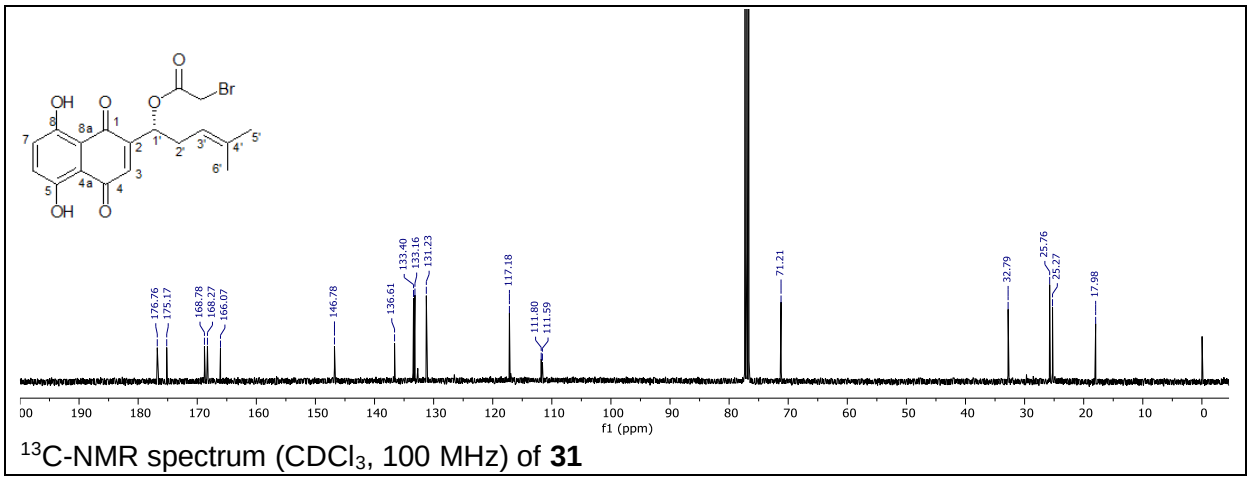
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **30**



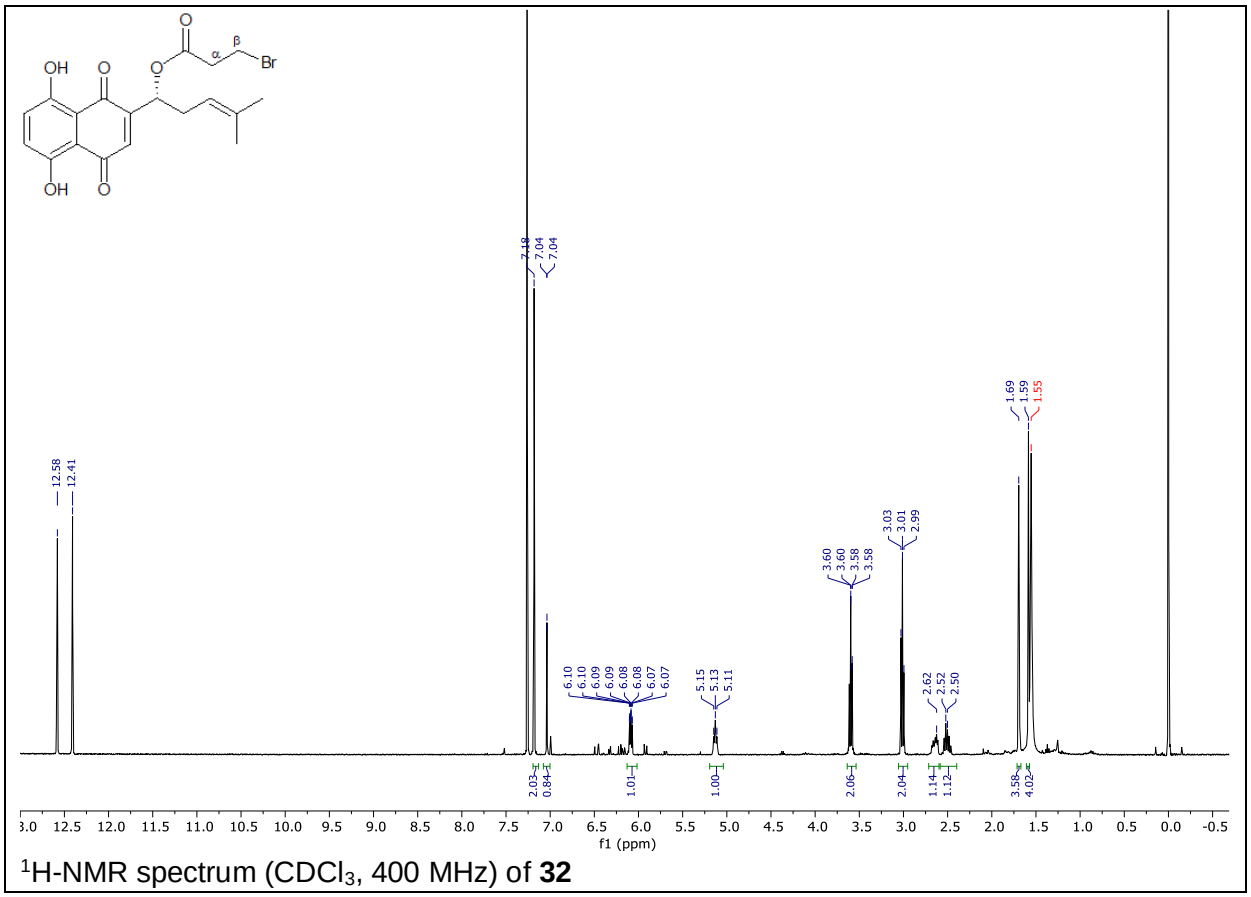
HMBC spectrum ($CDCl_3$, 100 MHz) of **31**



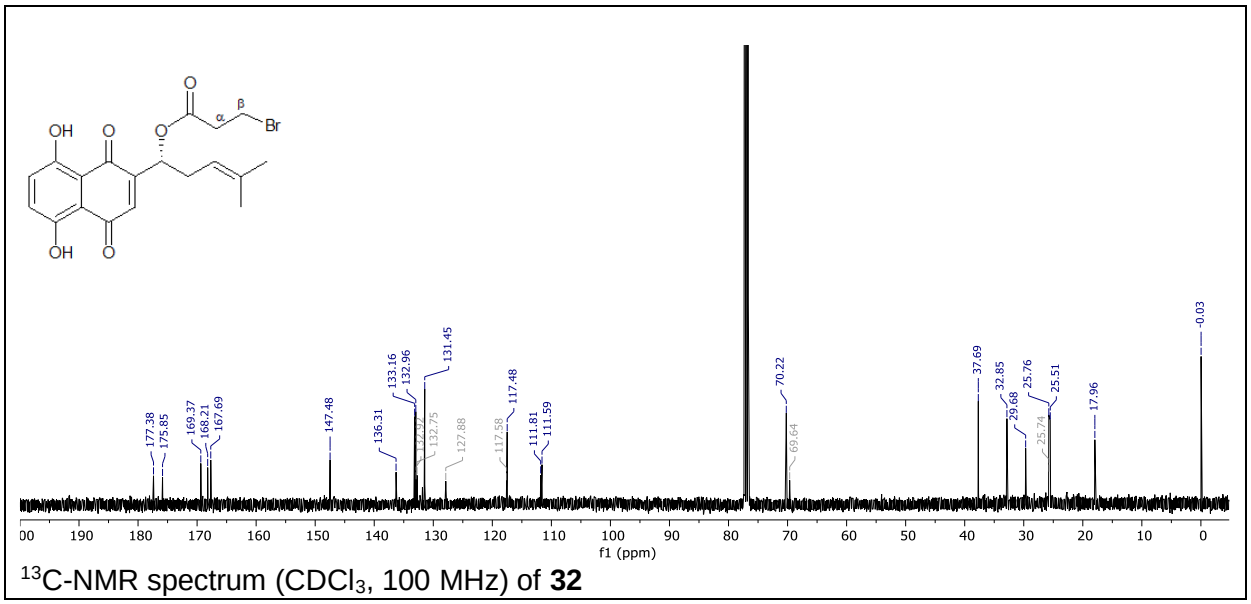
^{1}H-NMR spectrum ($CDCl_3$, 100 MHz) of **31**



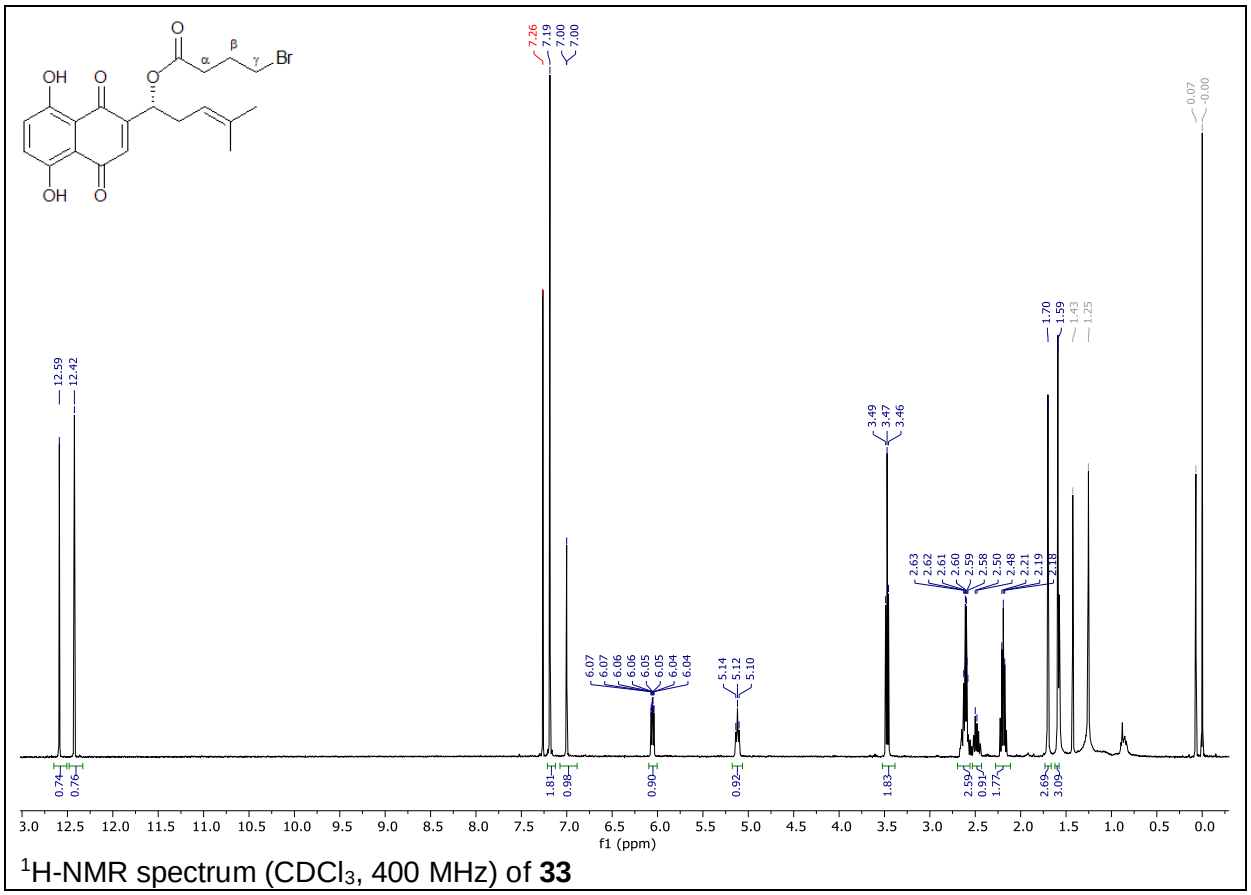
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **31**



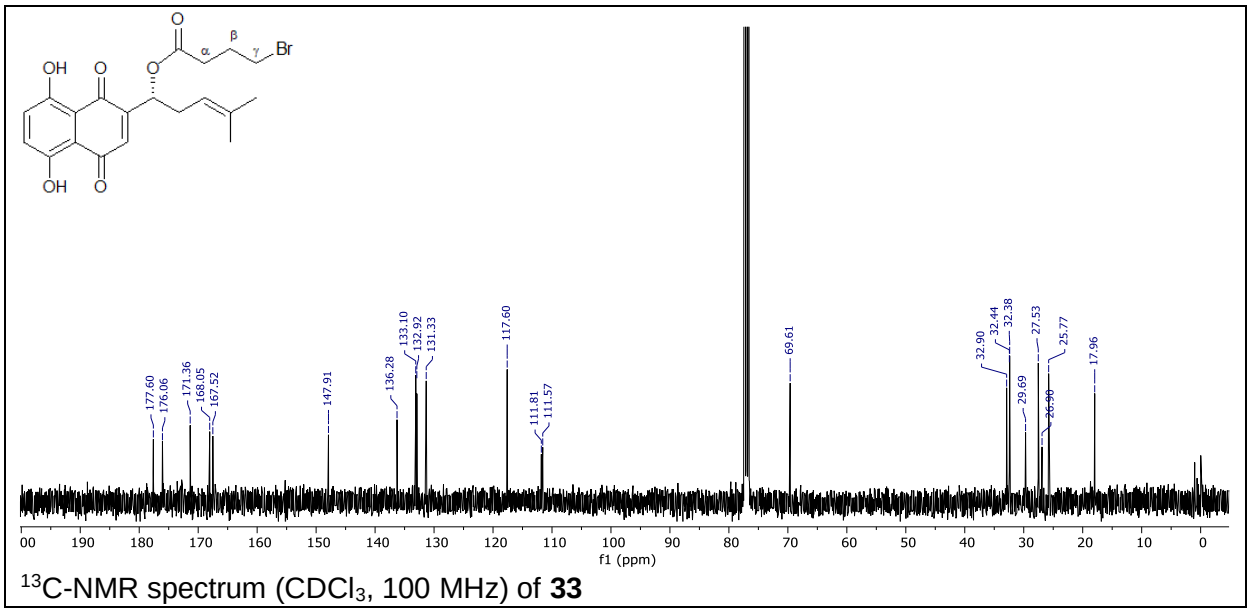
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **32**



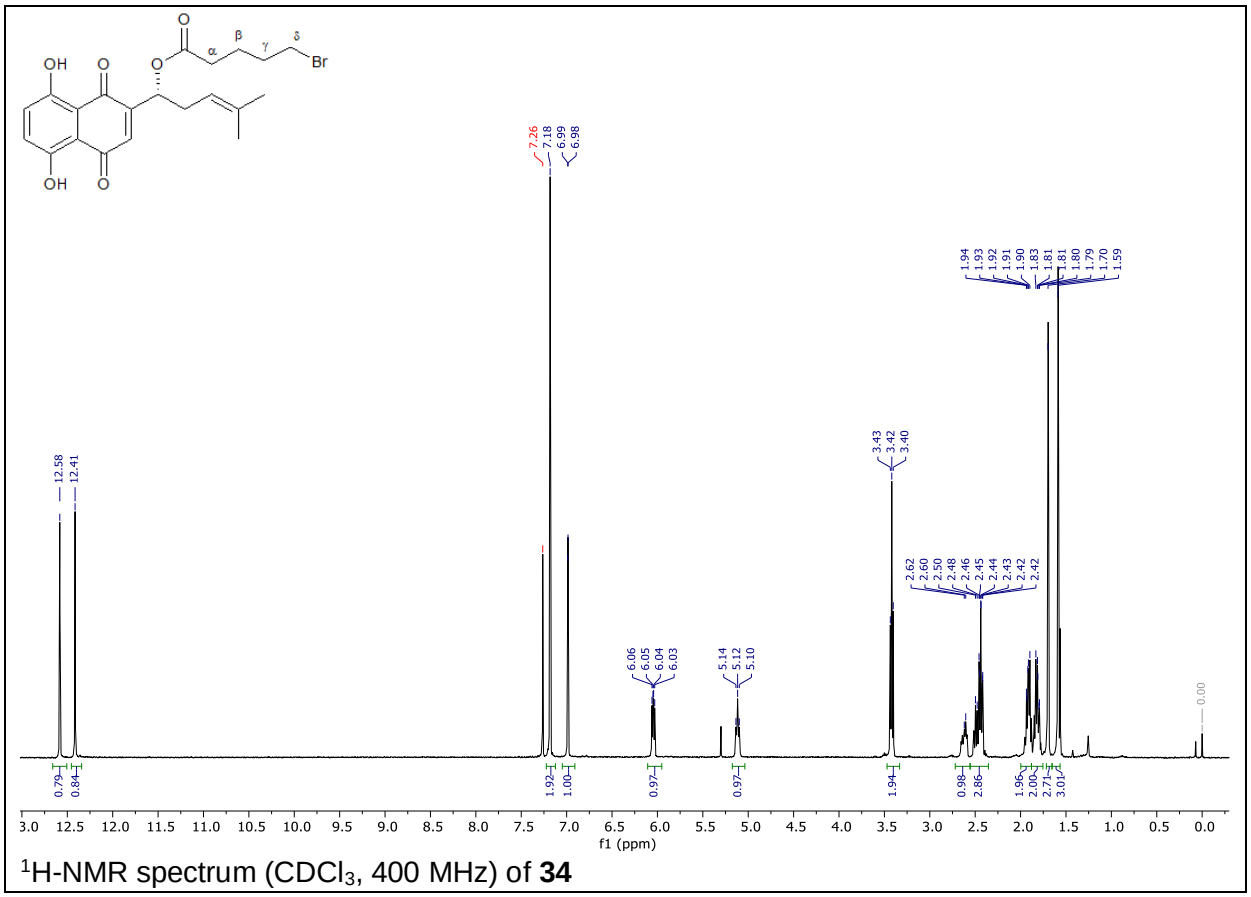
^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **32**



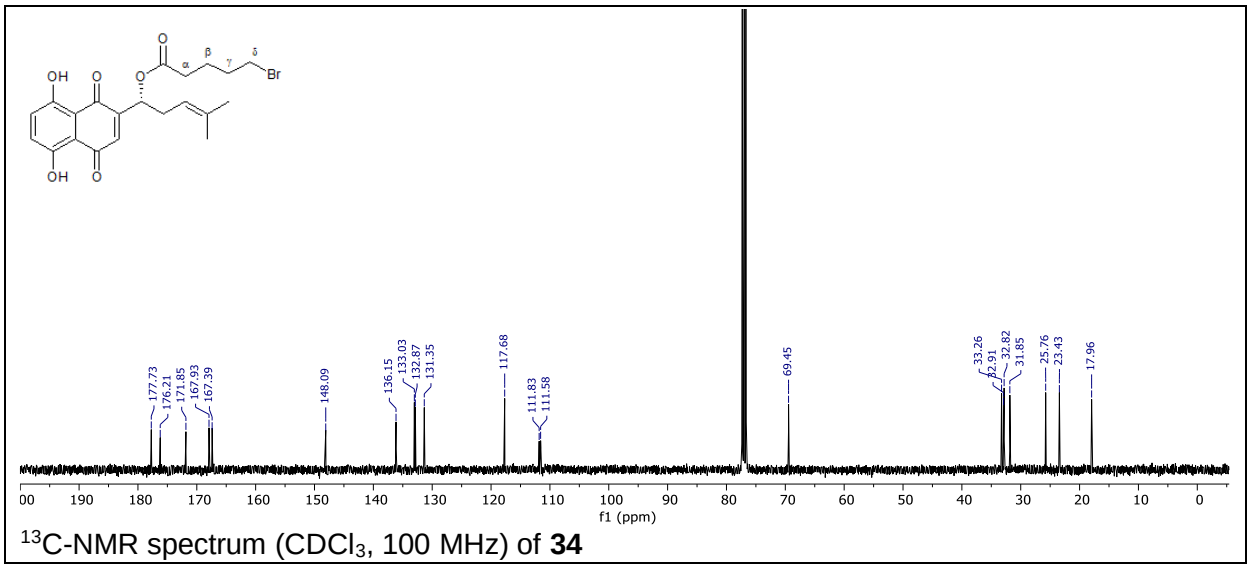
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **33**



^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **33**

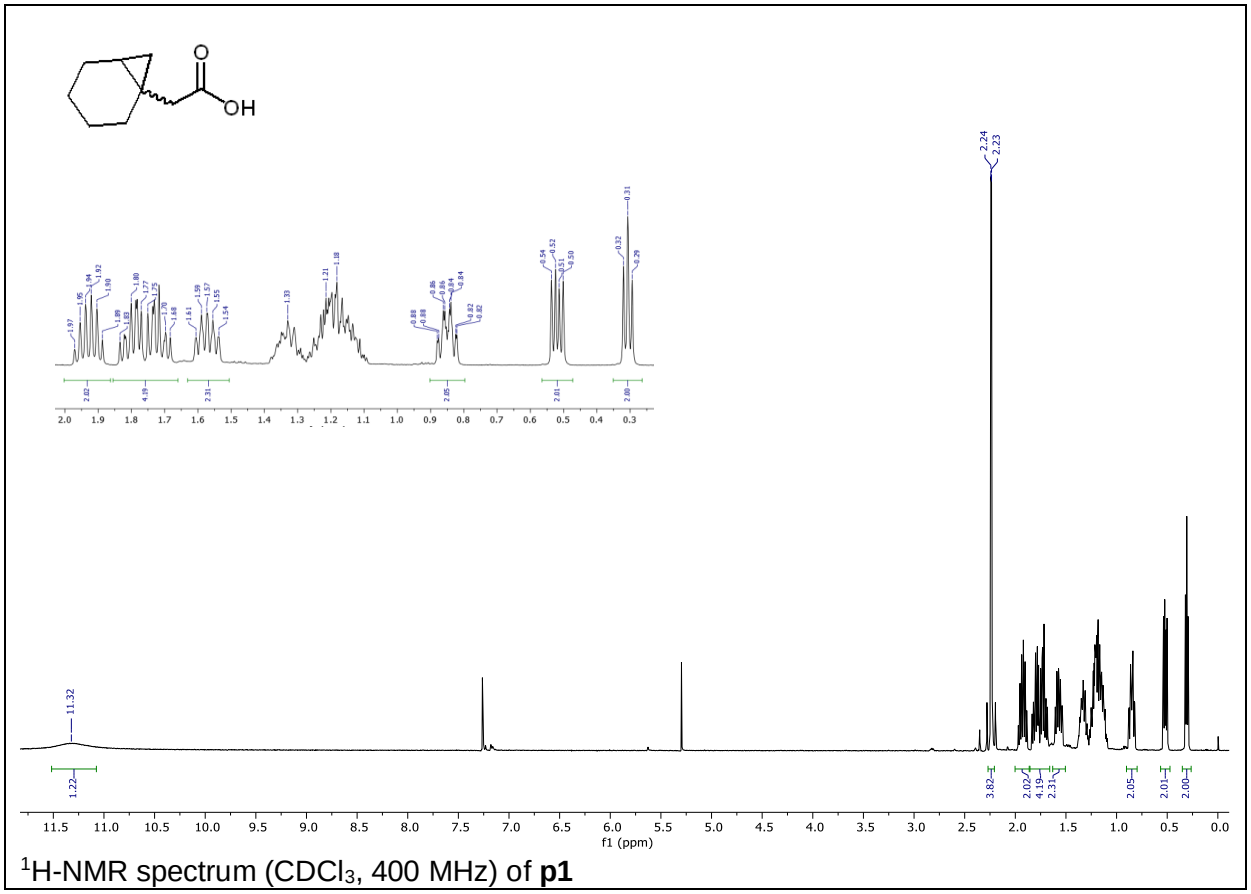


^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **34**

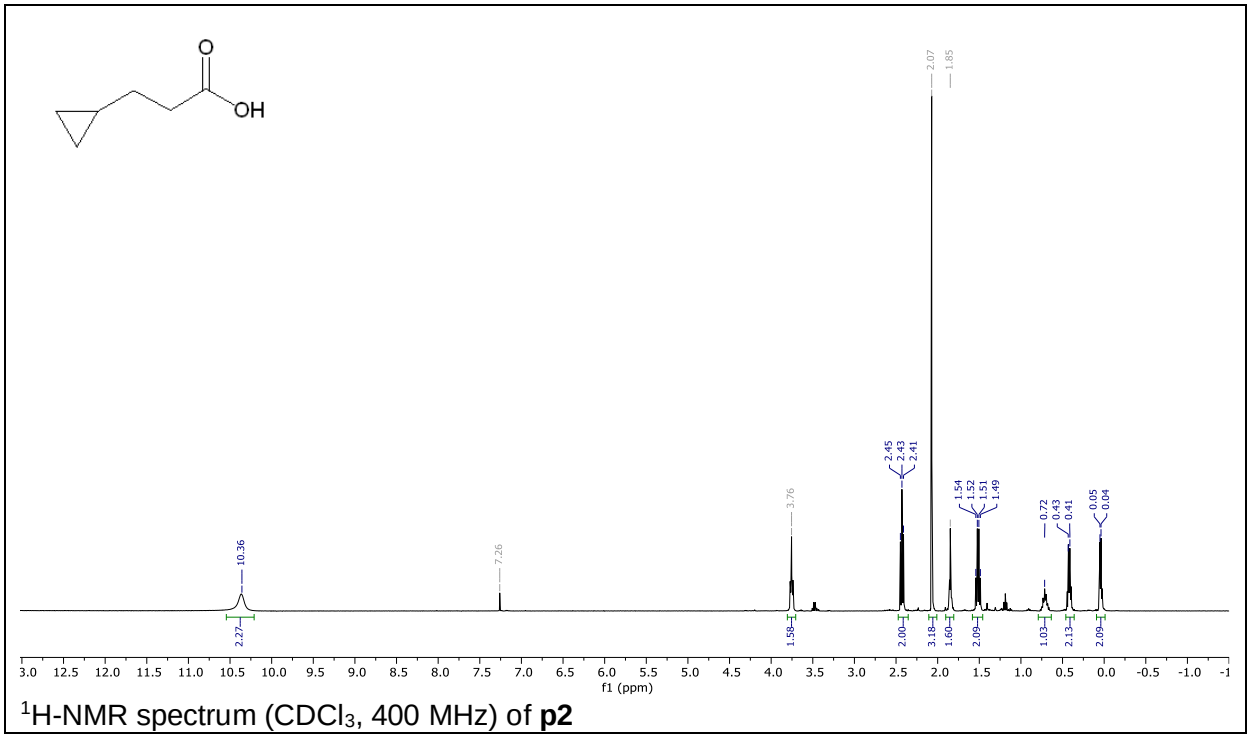


^{13}C-NMR spectrum ($CDCl_3$, 100 MHz) of **34**

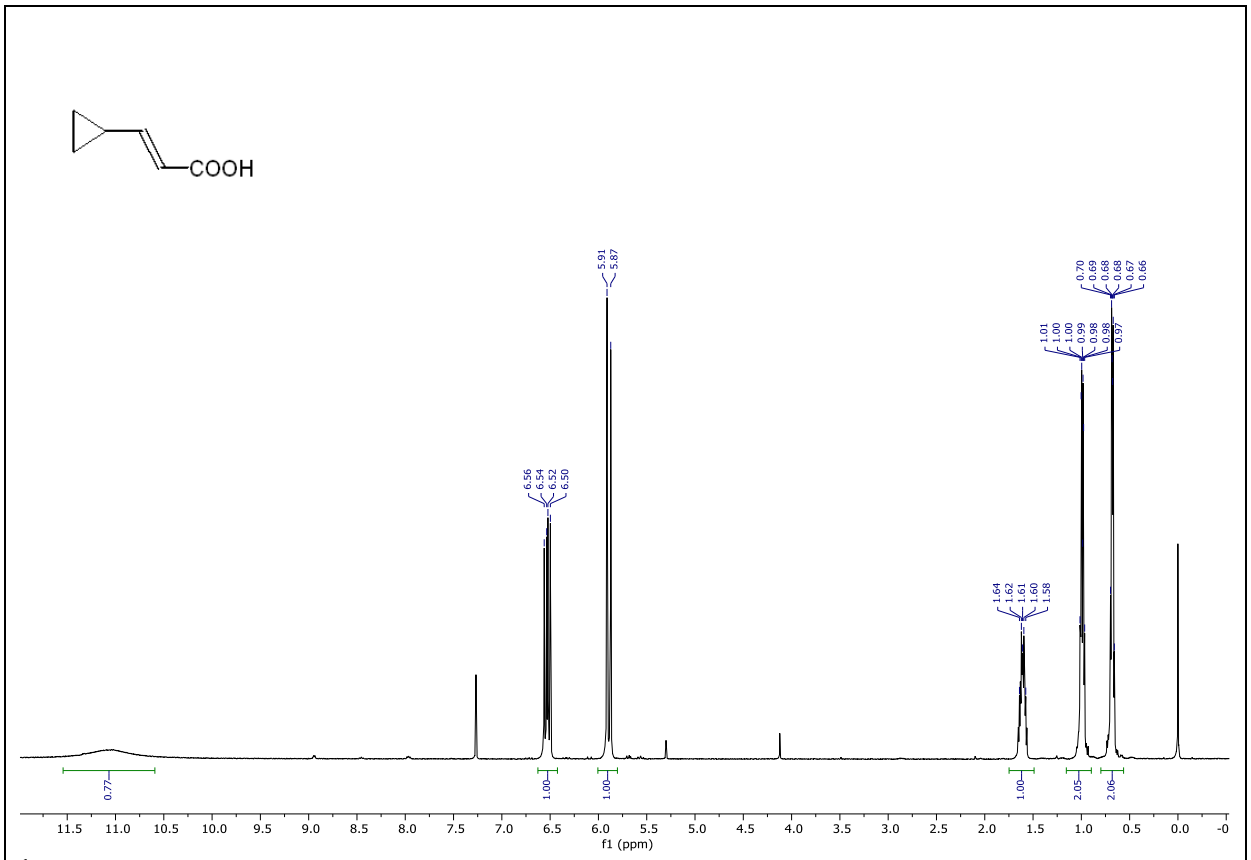
3. ^{1}H NMR spectra of precursor acids



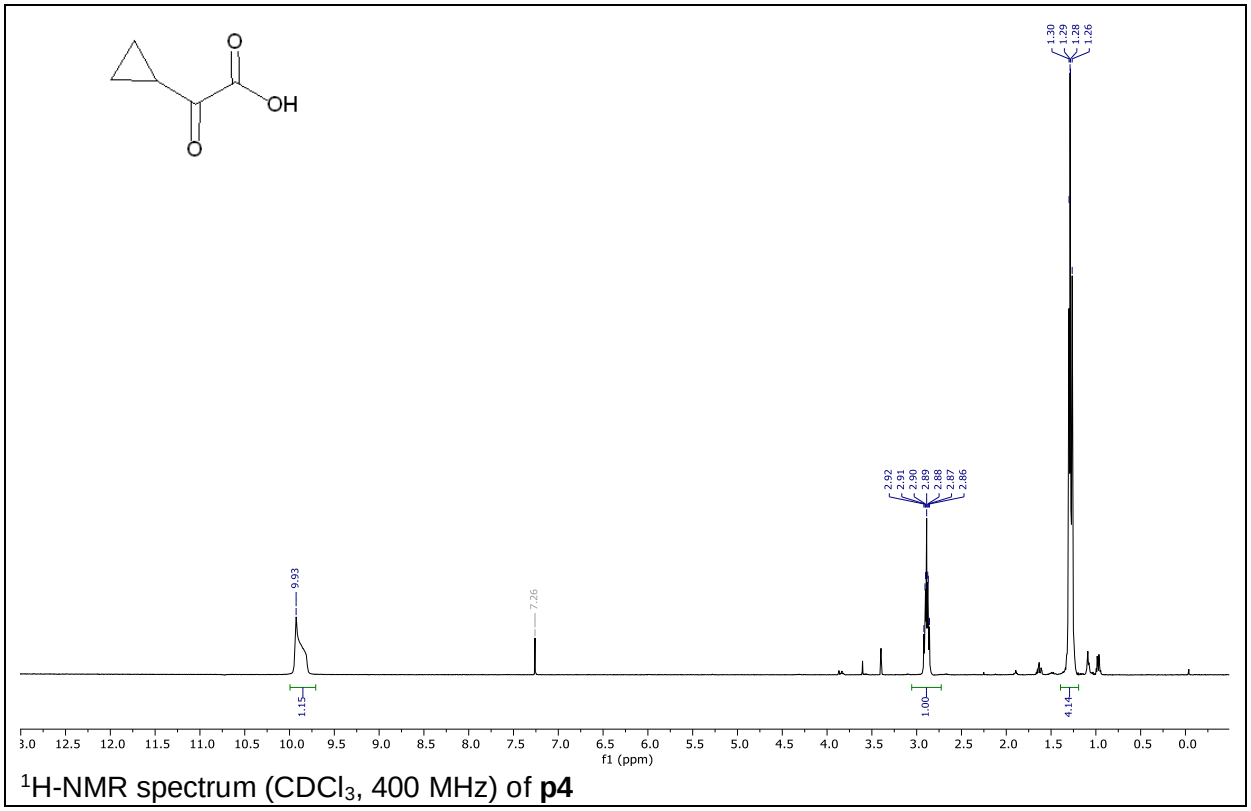
^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **p1**



^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **p2**



^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **p3**



^{1}H-NMR spectrum ($CDCl_3$, 400 MHz) of **p4**