

SUPPLEMENTARY INFORMATION

Cytotoxicity, Anti-diabeticity, and Phytochemical Investigation of Vietnamese *Euphorbia tithymaloides* Linn. (Euphorbiaceae)

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TABLE OF CONTENTS:

Figure S1–S8. ¹ H-NMR, ¹³ C-NMR, COSY, HSQC, HMBC (total & sketched), NOESY, and MS spectra of compound P1 (in Acetone- <i>d</i> ₆)	S2–S9
Figure S9–S19. ¹ H-NMR, ¹³ C-NMR (total & sketched), COSY, HSQC, HMBC, NOESY, MS spectra (in CDCl ₃), and structural novelty check for compound P2	S10–S20
Figure S20–S33. ¹ H-NMR, ¹³ C-NMR (total & sketched), COSY, HSQC, HMBC, NOESY (total & sketched), and MS spectra of compound P3 (in Acetone- <i>d</i> ₆)	S21–S34
Figure S34–S41. ¹ H-NMR, ¹³ C-NMR, COSY, HSQC, HMBC (total & sketched), NOESY, MS spectra (in CDCl ₃), and structural novelty check for compound P4	S35–S42
Figure S42–S51. ¹ H-NMR, ¹³ C-NMR, COSY, HSQC, HMBC (total & sketched), NOESY, MS spectra (in CDCl ₃), and structural novelty check for compound P5	S43–S52

Figure S1. $^1\text{H-NMR}$ (600 MHz, Acetone- d_6) spectrum of compound P1

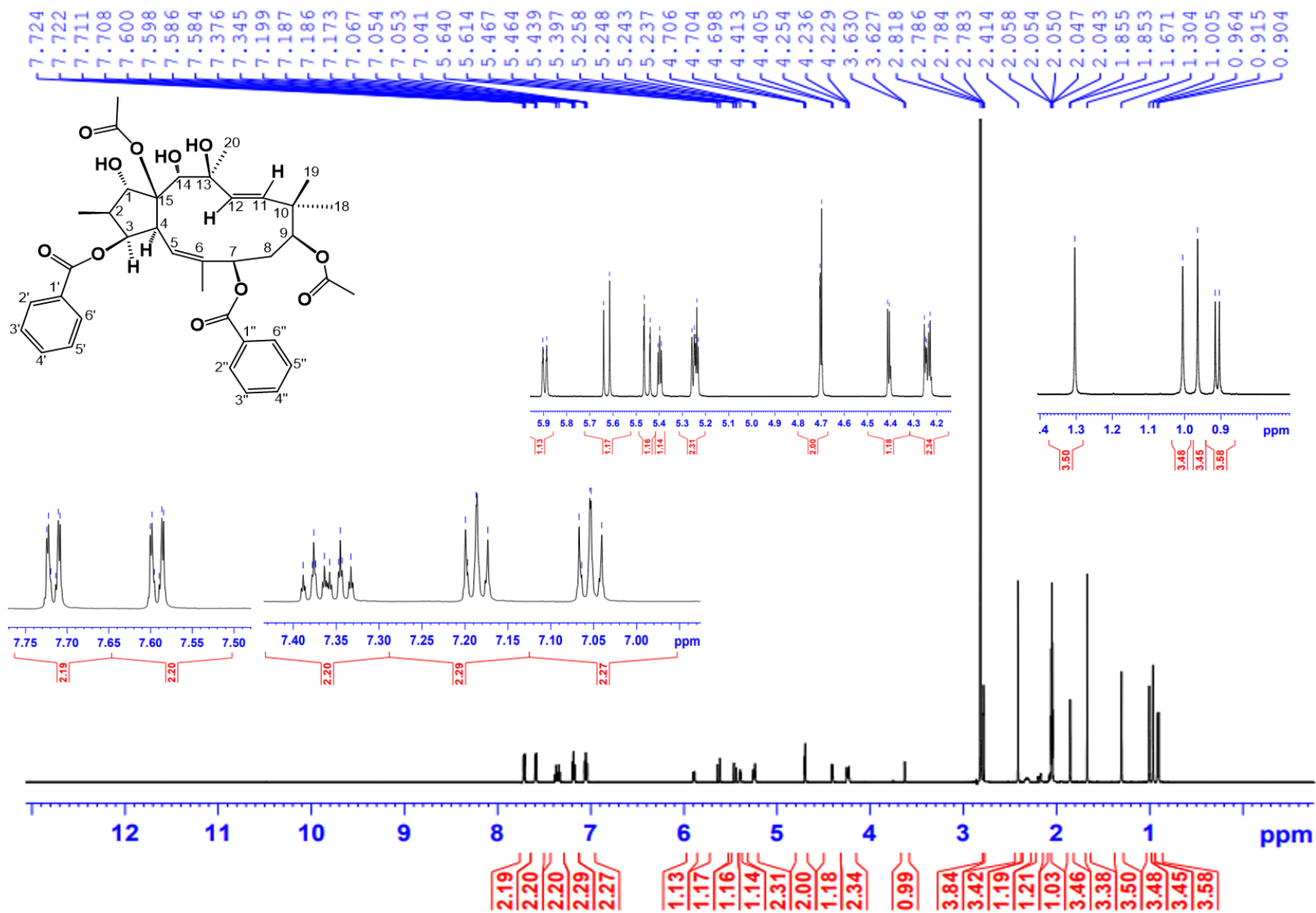


Figure S2. ^{13}C -NMR (125 MHz, Acetone- d_6) spectrum of compound P1

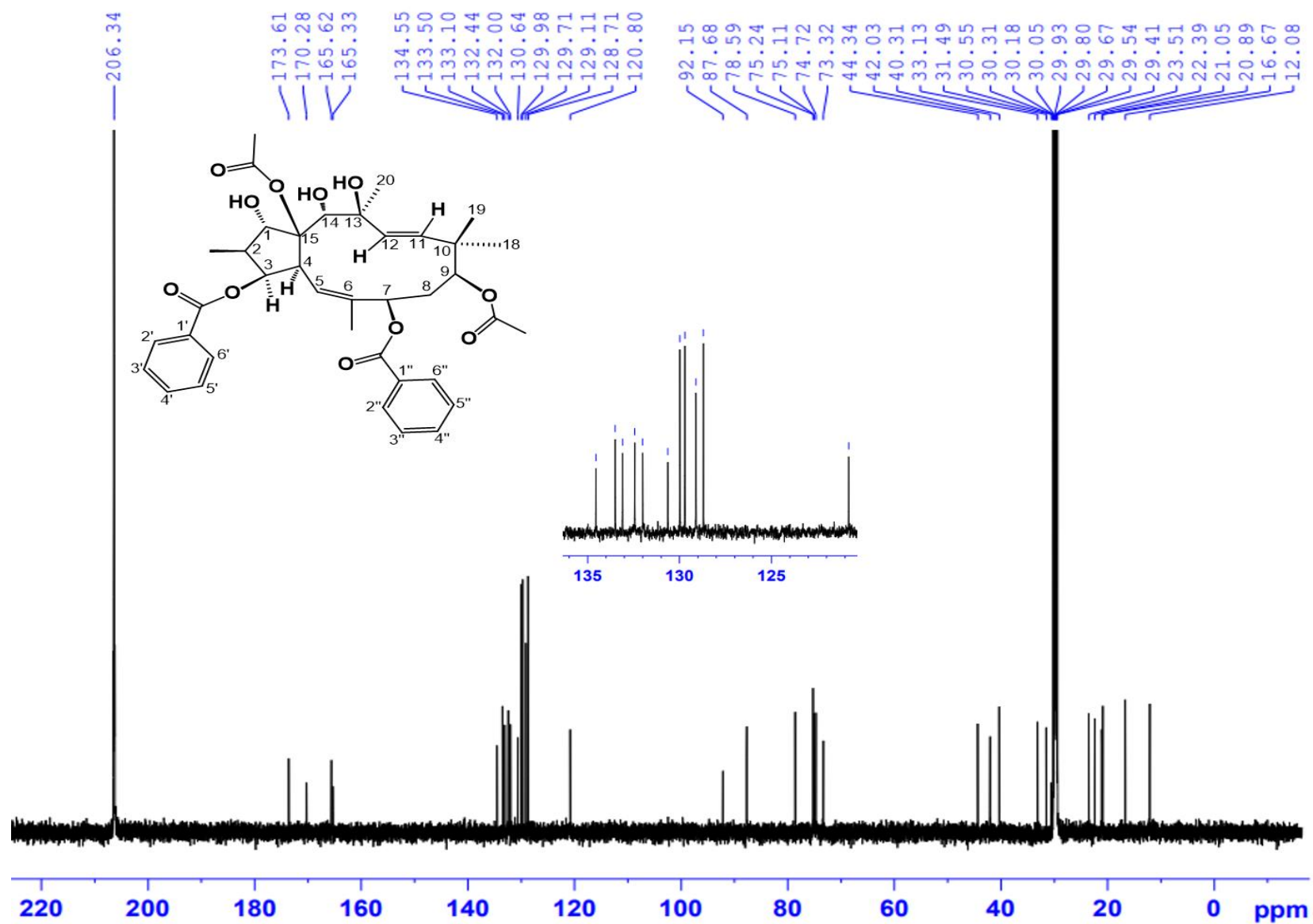


Figure S4. HSQC (Acetone- d_6) spectrum of compound P1

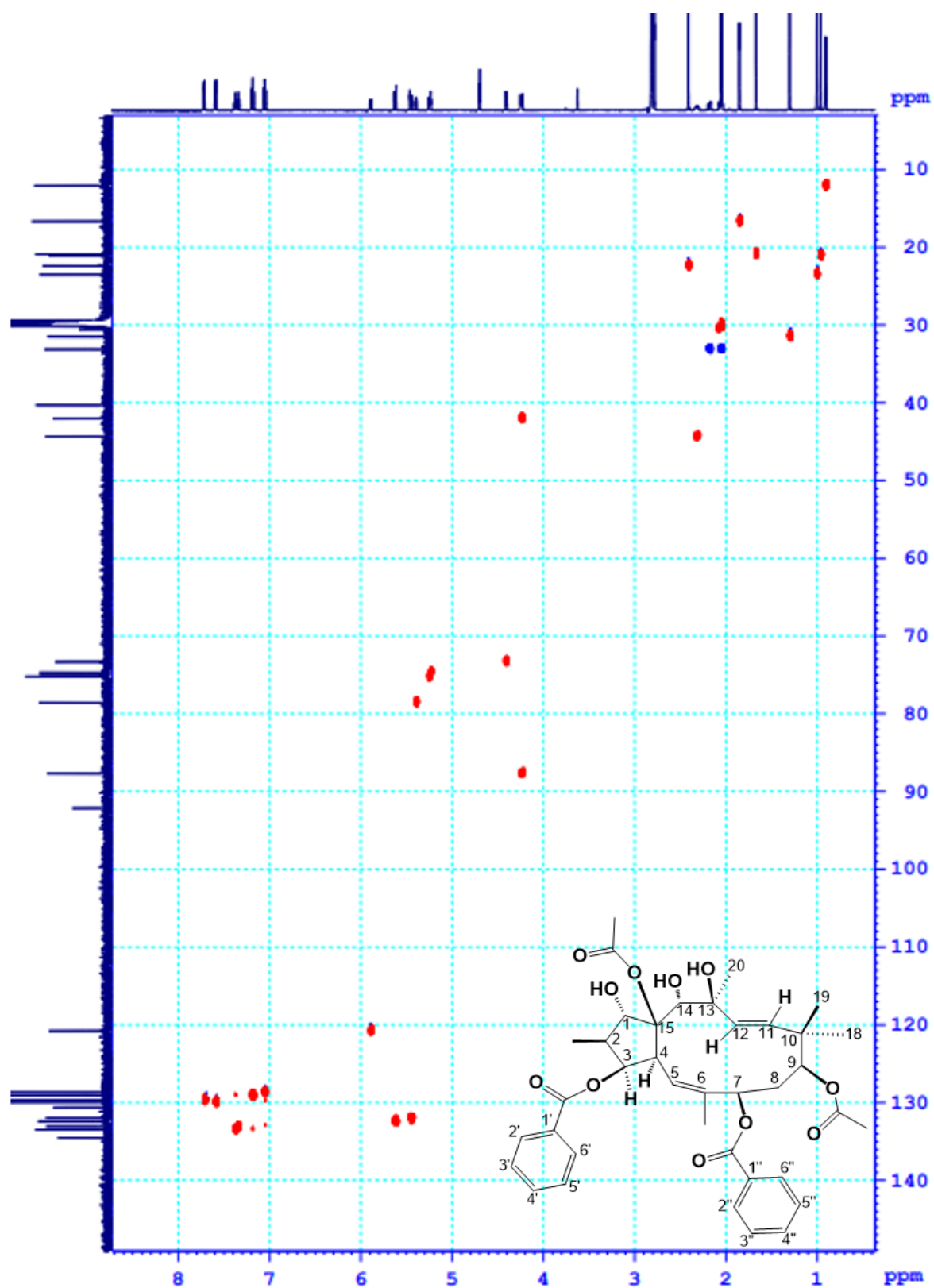


Figure S5. HMBC (Acetone- d_6) spectrum (total) of compound P1

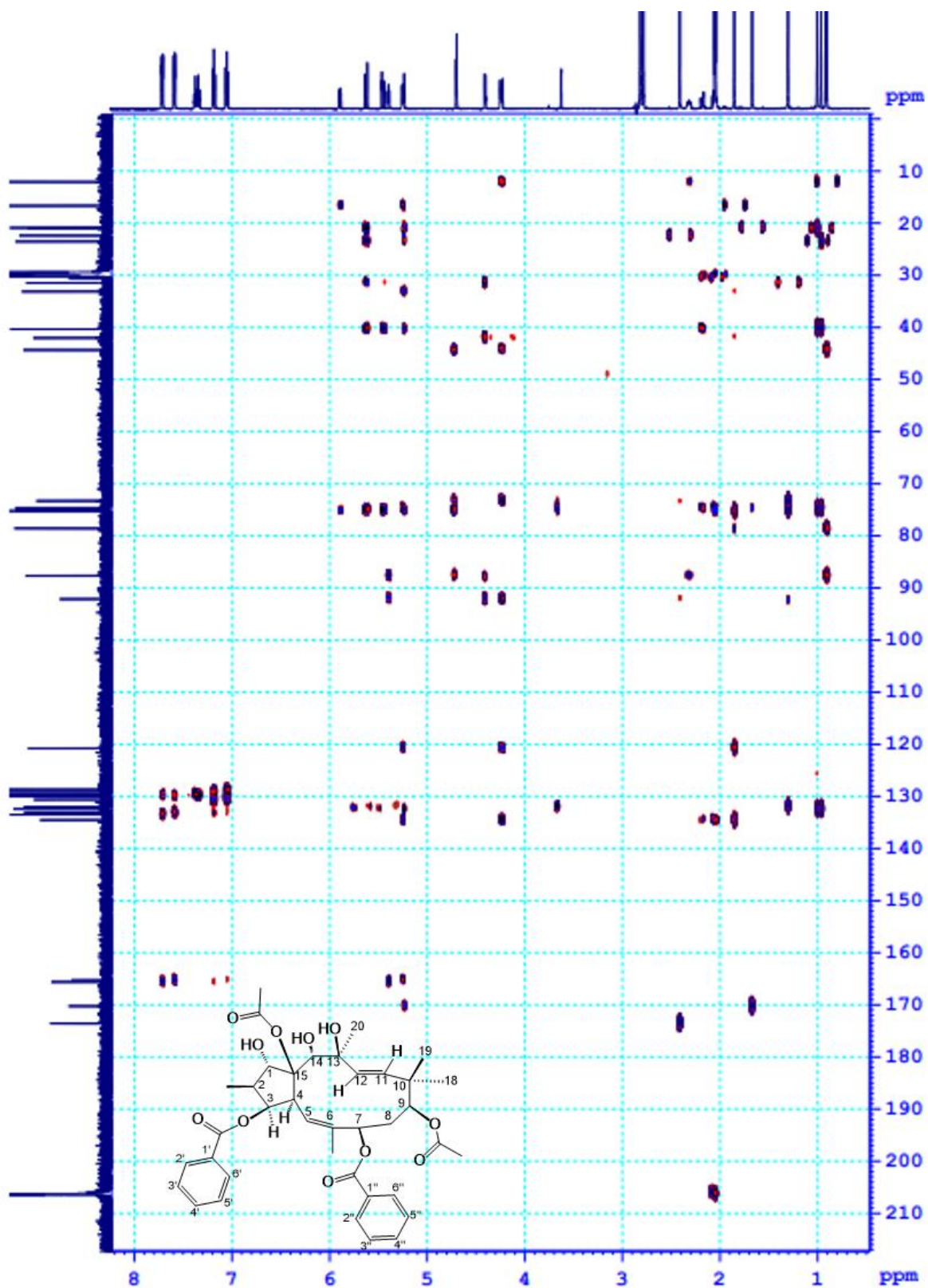


Figure S6. HMBC (Acetone- d_6) spectrum (sketched) of compound P1

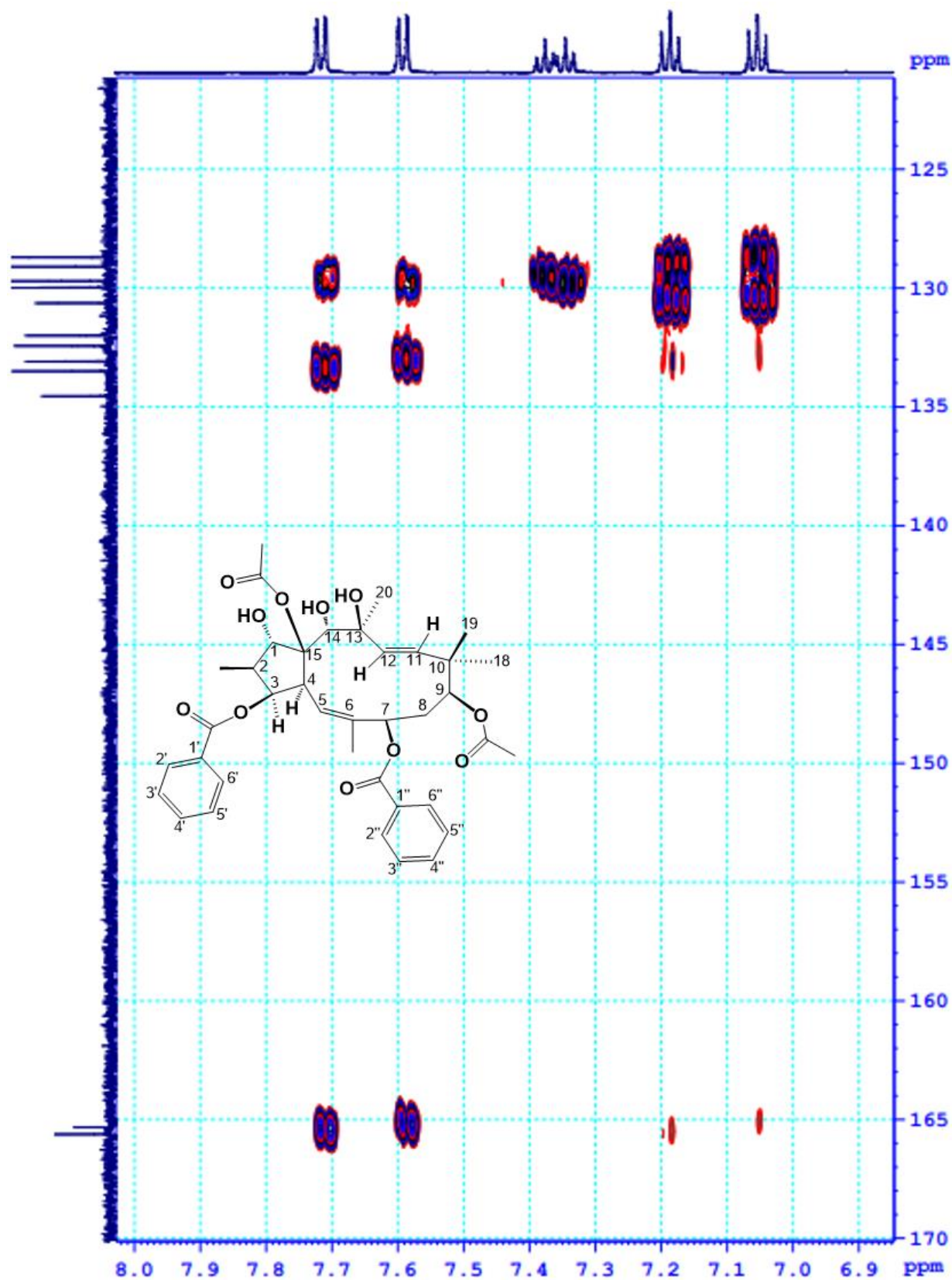


Figure S7. NOESY (Acetone- d_6) spectrum of compound P1

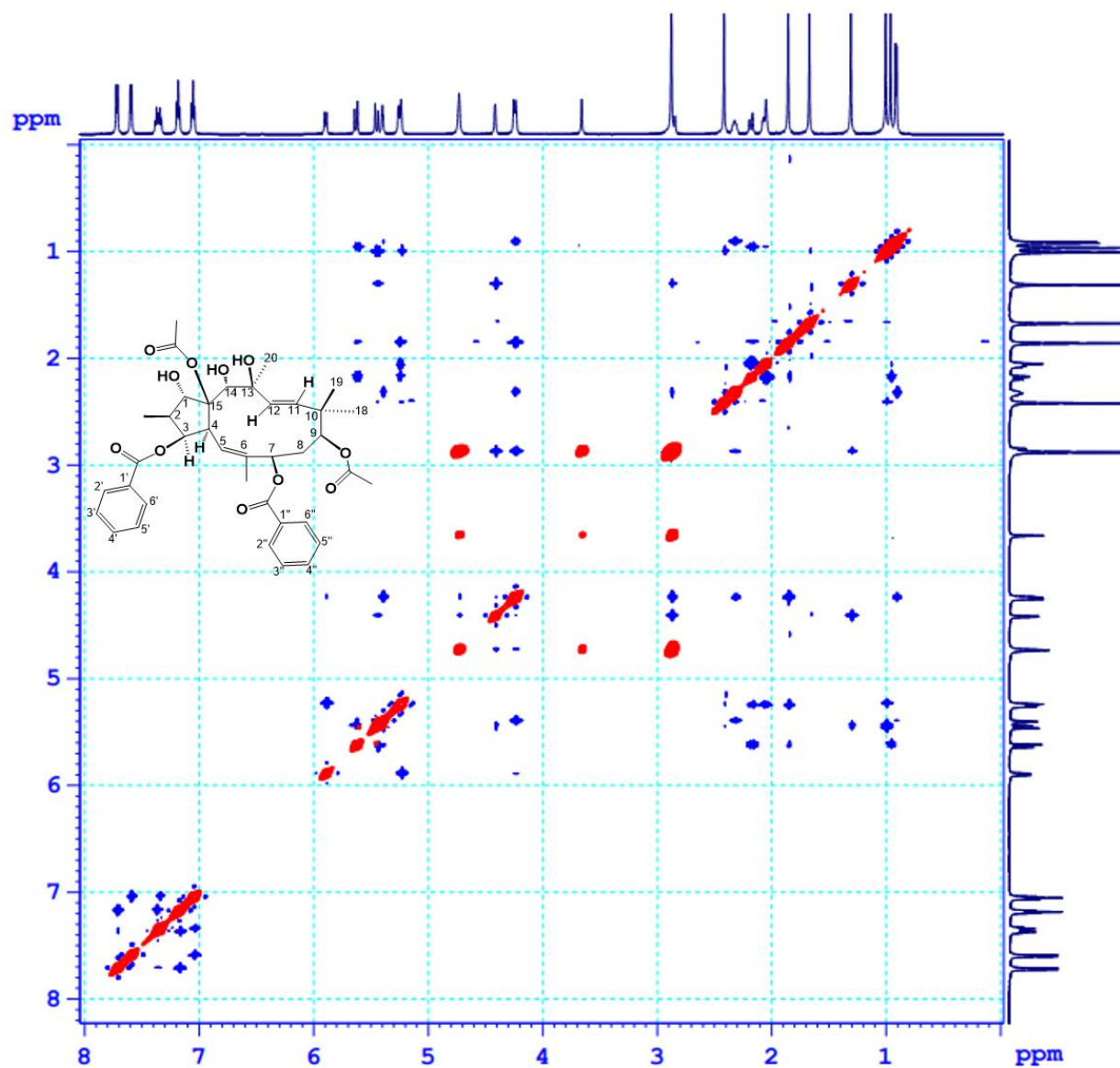


Figure S8. MS spectrum of compound P1 (Acetone-*d*₆)

Sample Name	P1	Position	P1-B4	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	AS1.d
ACQ Method	Cot ngan - MSMS_Pos1.m	Comment		Acquired Time	21/07/2022 1:12:50 PM

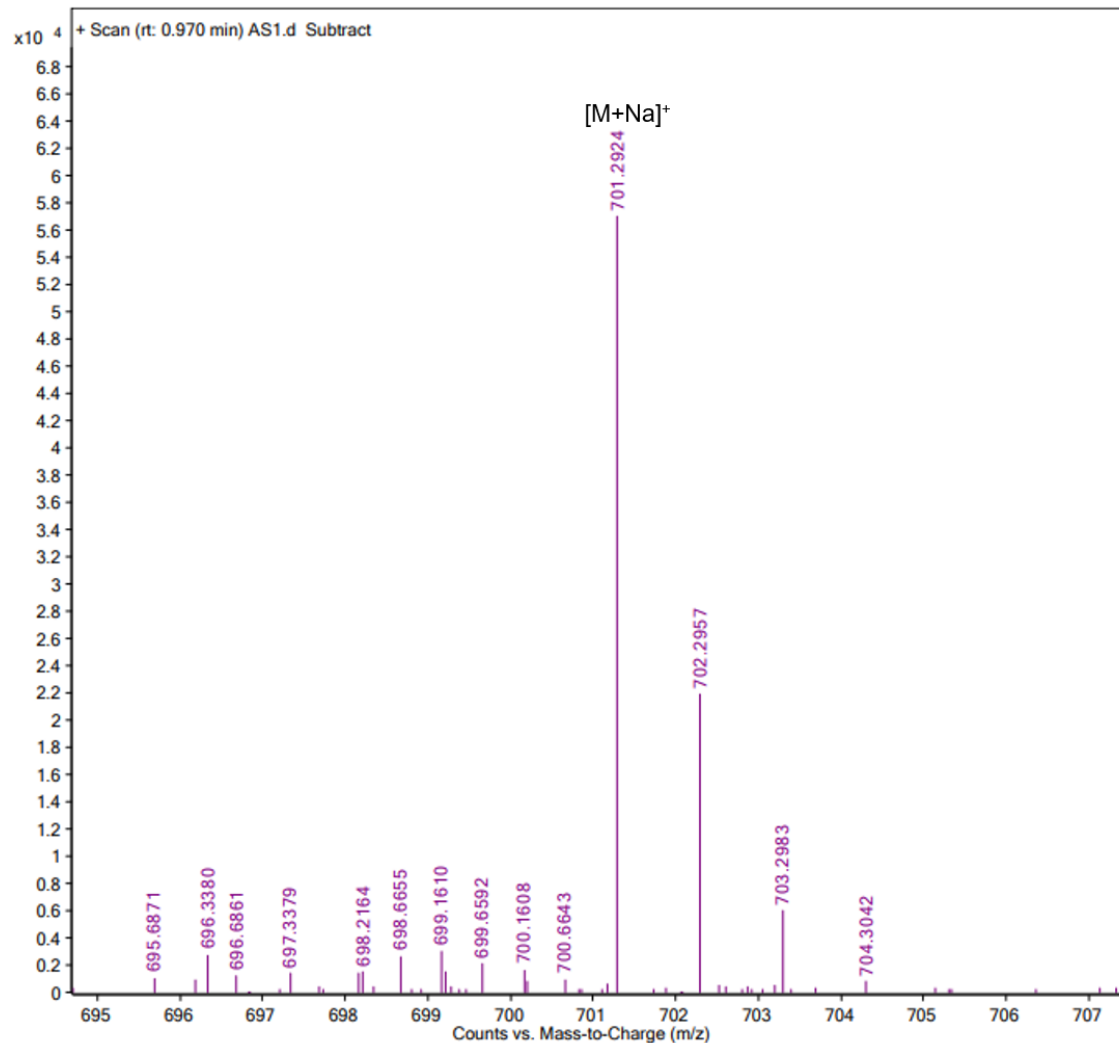


Figure S9. ¹H-NMR (600 MHz, CDCl₃) spectrum (total) of compound P2

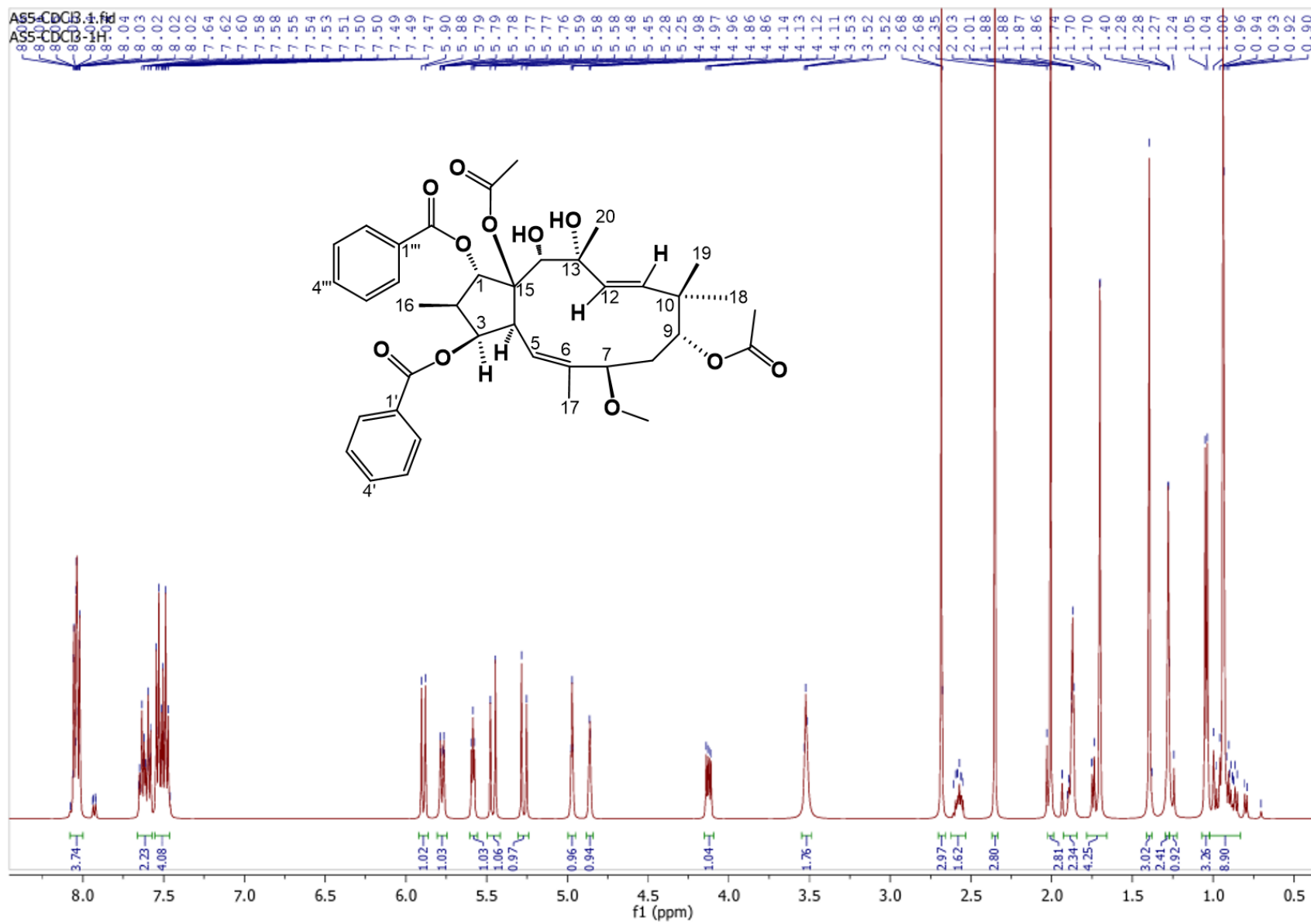


Figure S10. $^1\text{H-NMR}$ (600 MHz, CDCl_3) spectrum (sketched) of compound **P2**

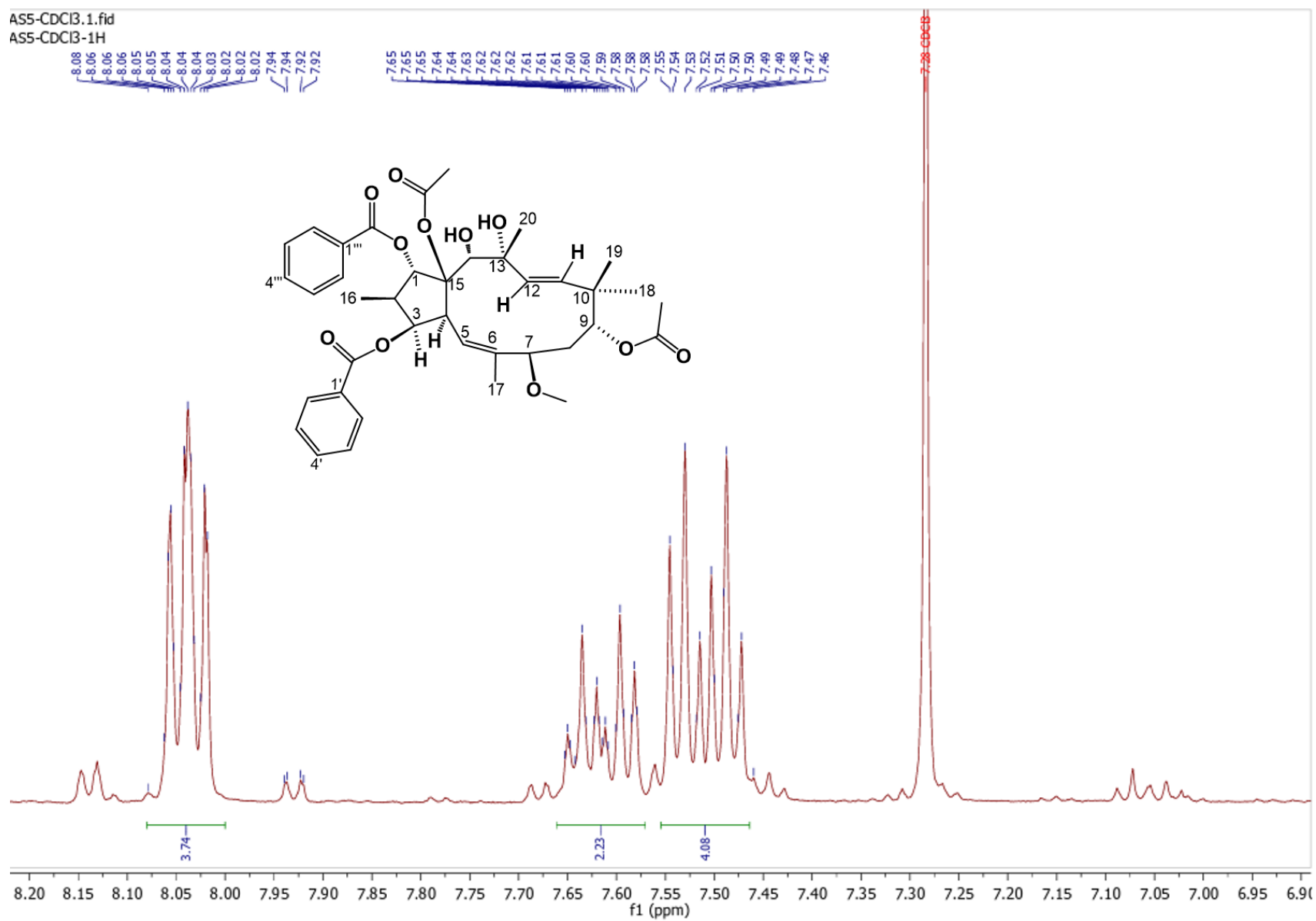


Figure S11. $^1\text{H-NMR}$ (600 MHz, CDCl_3) spectrum (sketched) of compound P2

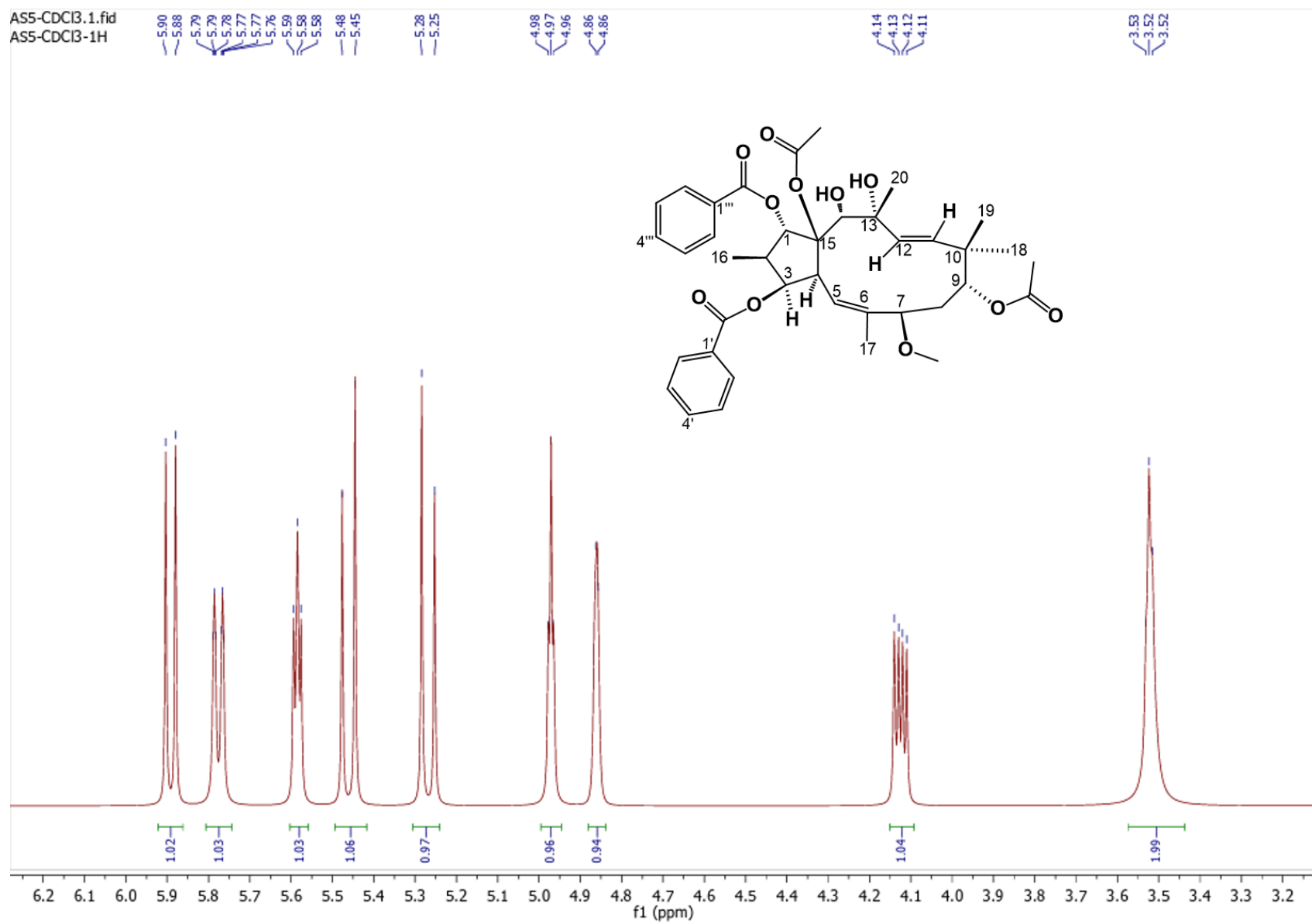


Figure S12. $^1\text{H-NMR}$ (600 MHz, CDCl_3) spectrum (sketched) of compound P2

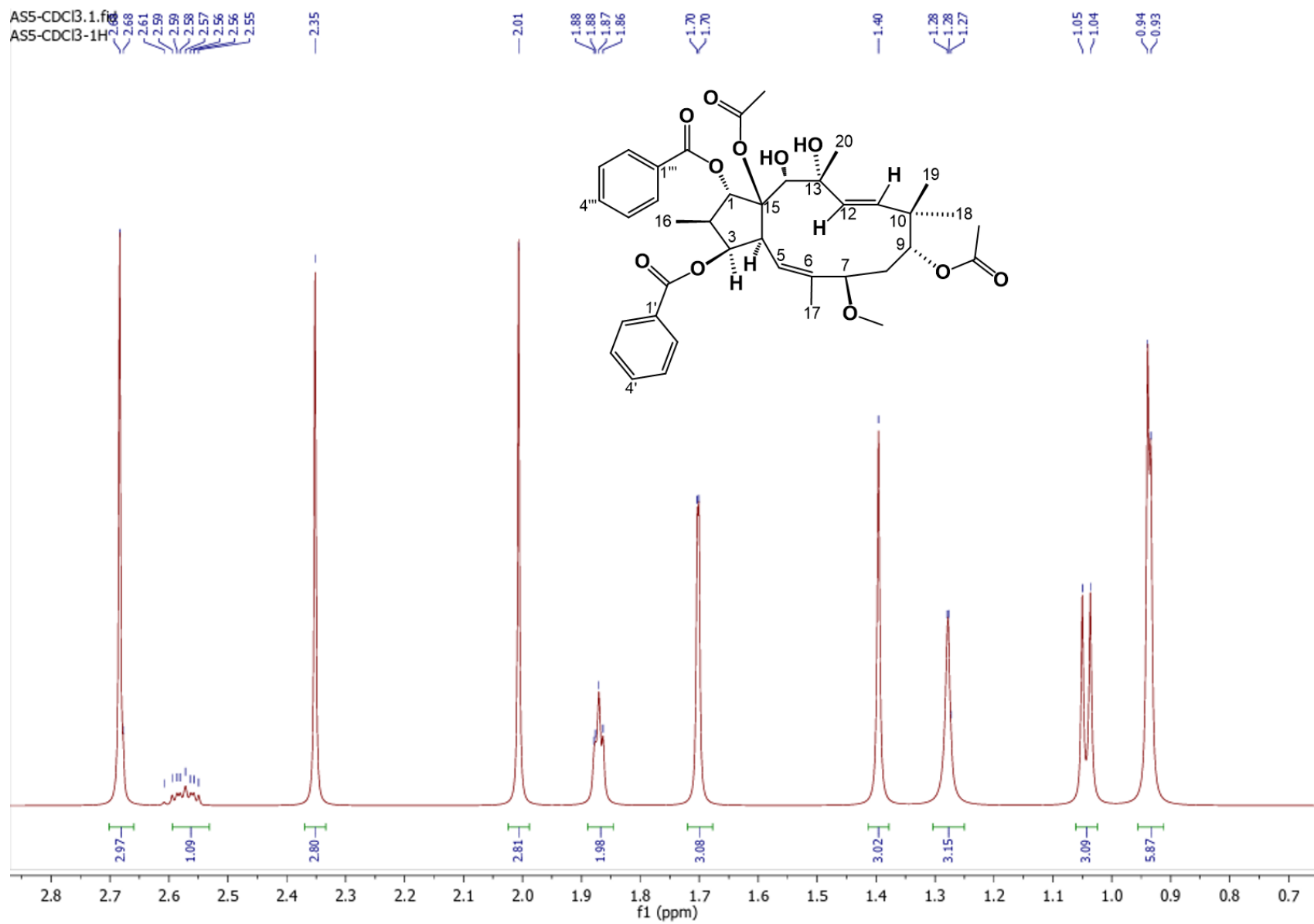


Figure S13. ^{13}C -NMR (125 MHz, CDCl_3) spectrum of compound P2

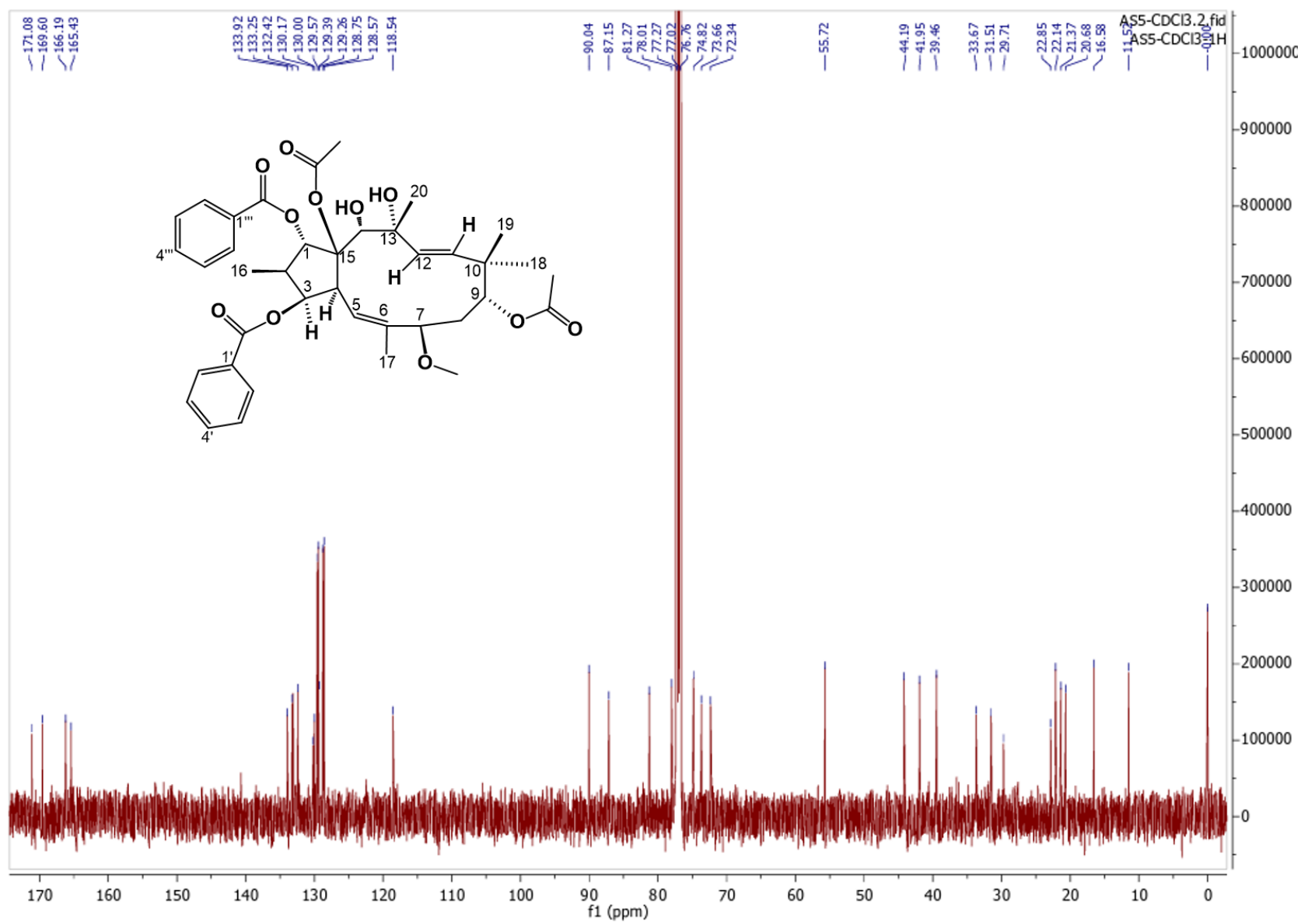


Figure S14. COSY (CDCl₃) spectrum of compound P2

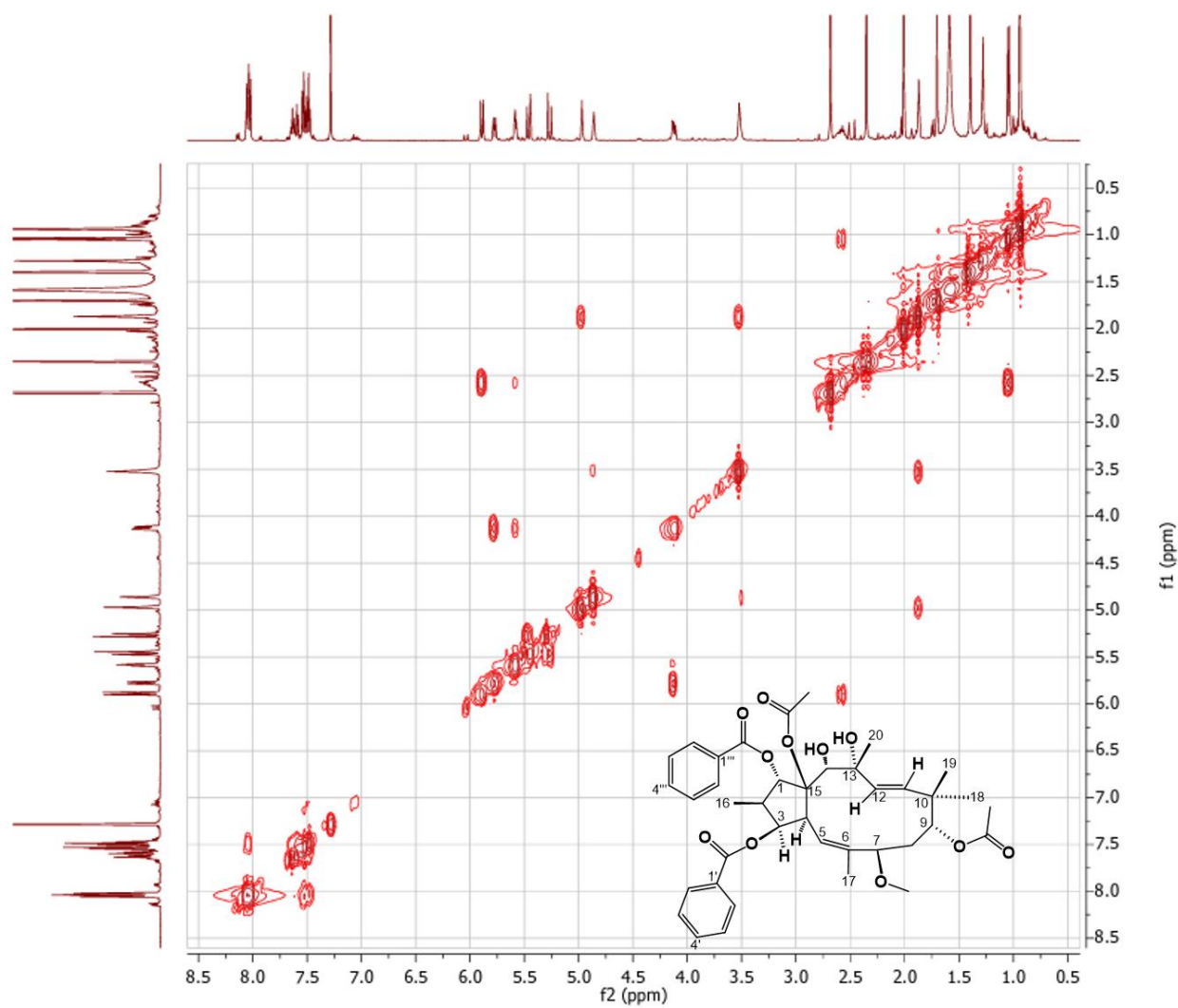


Figure S15. HSQC (CDCl₃) spectrum of compound P2

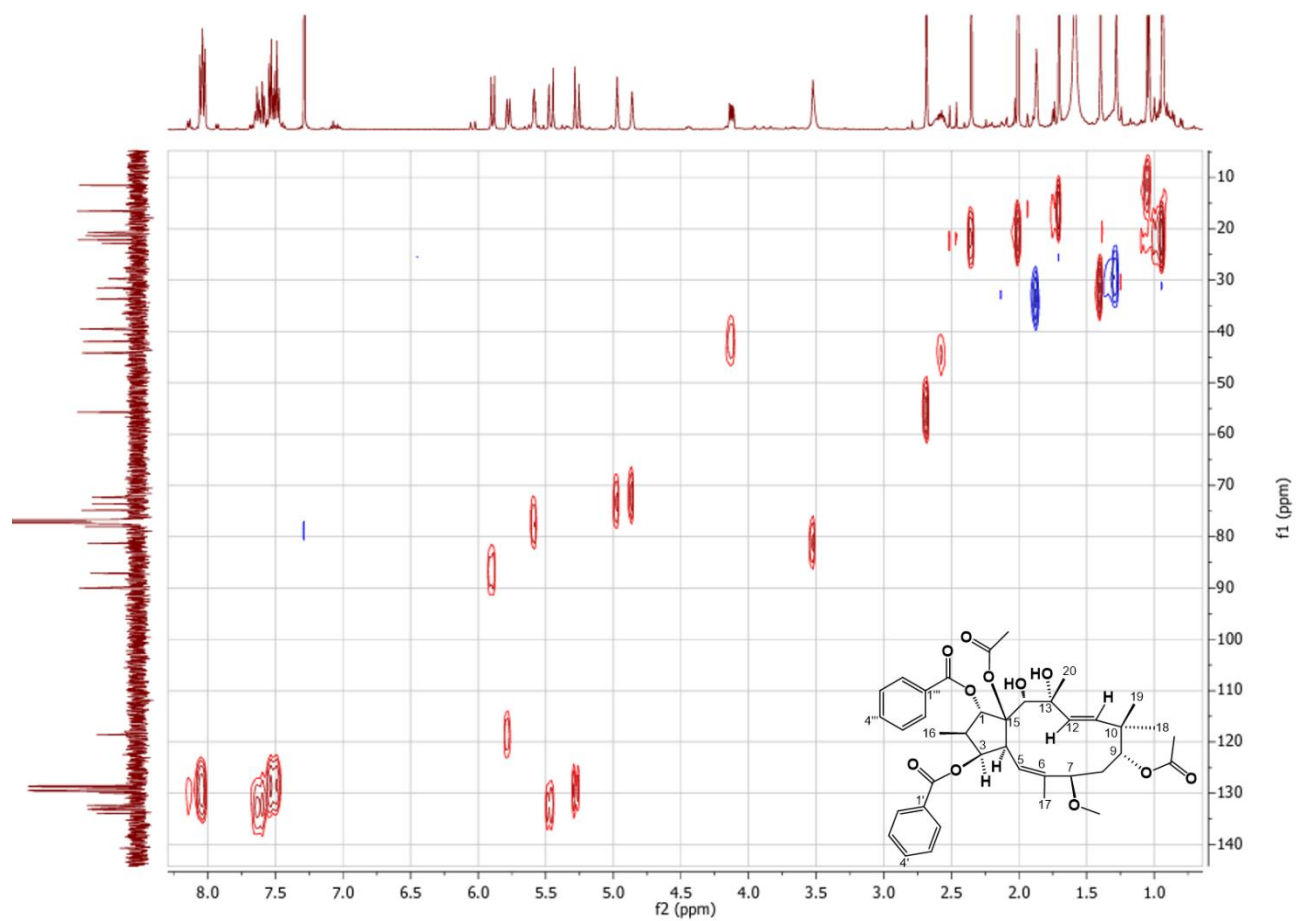


Figure S16. HMBC (CDCl₃) spectrum of compound P2

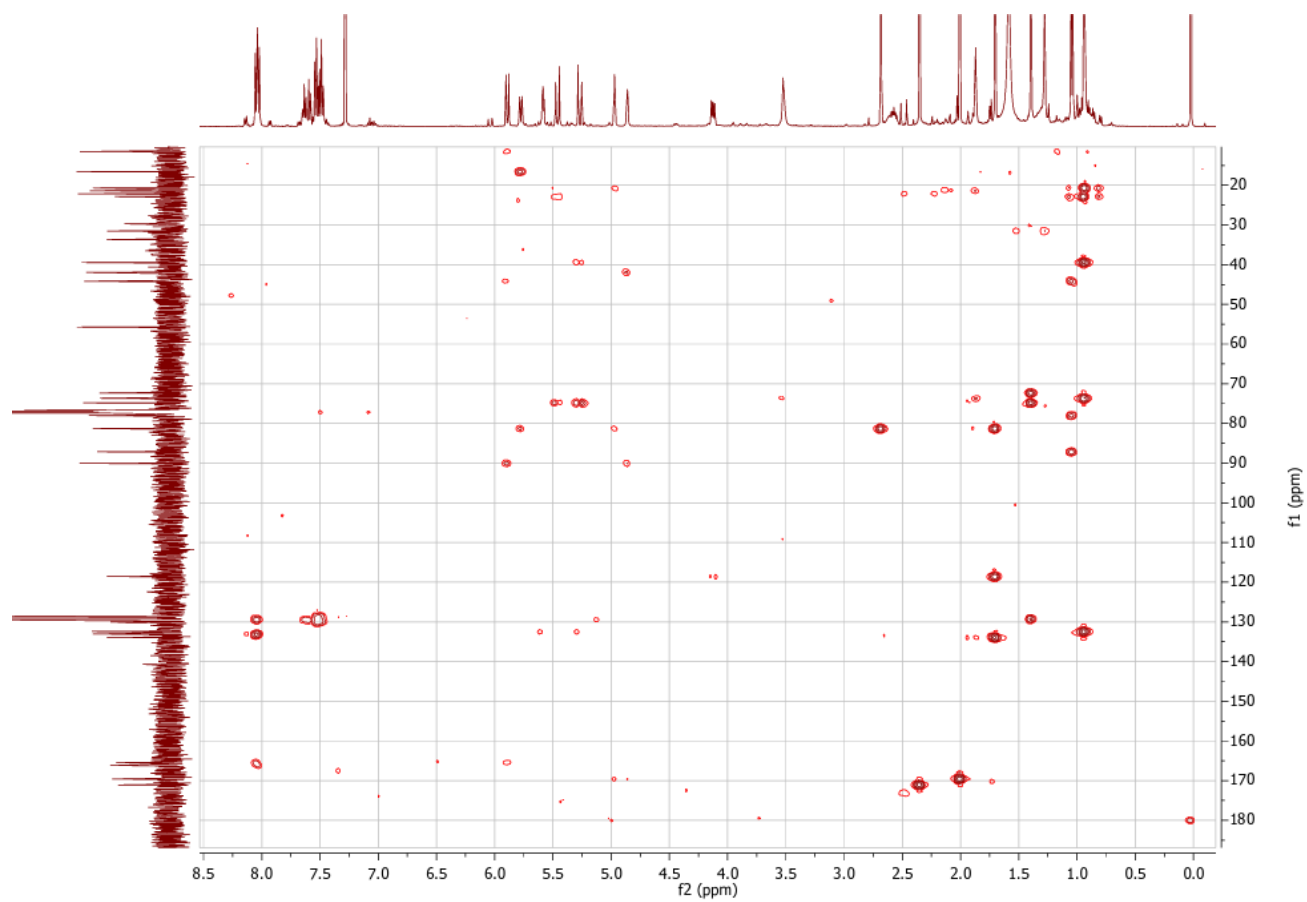


Figure S17. NOESY (CDCl₃) spectrum of compound P2

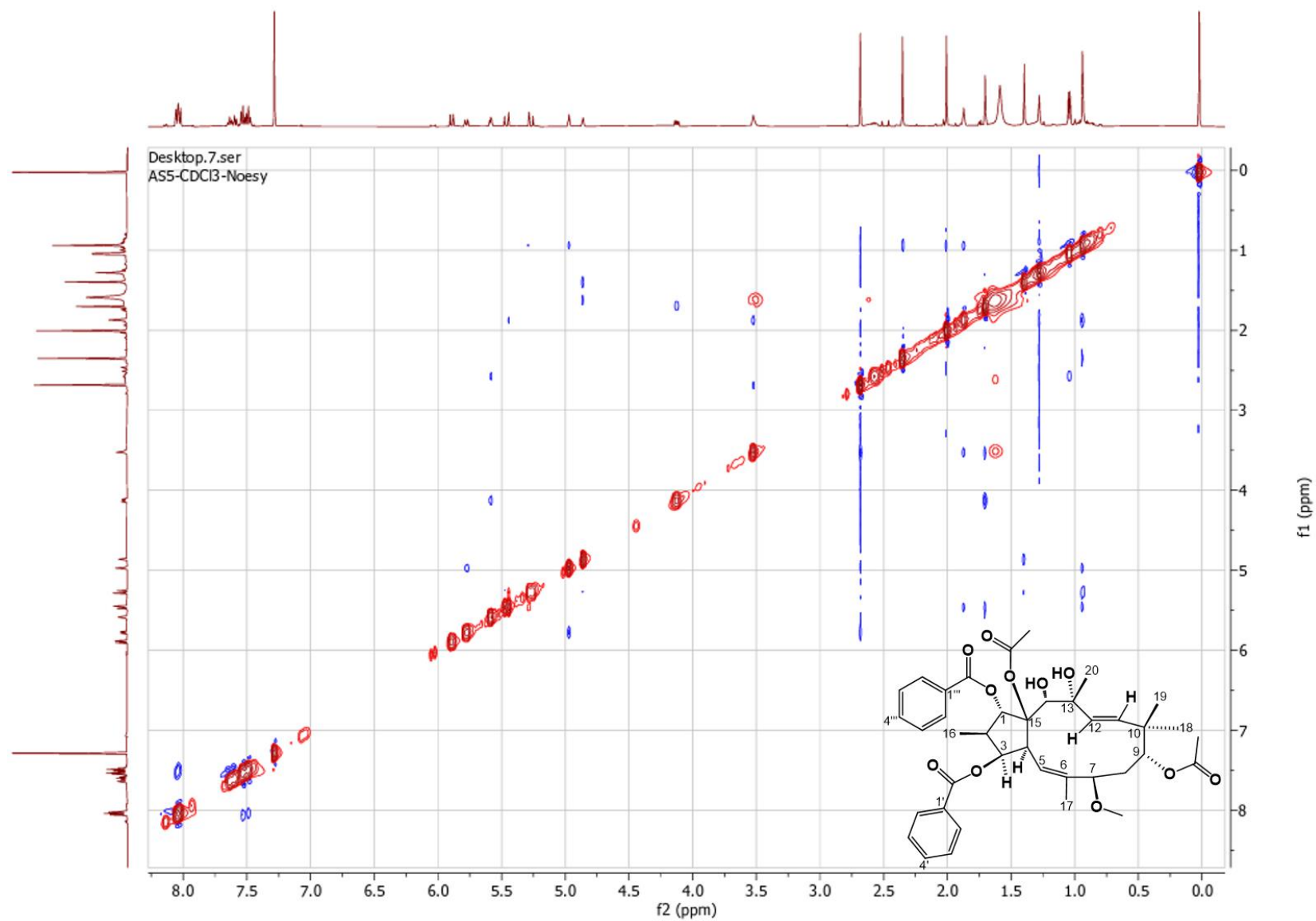
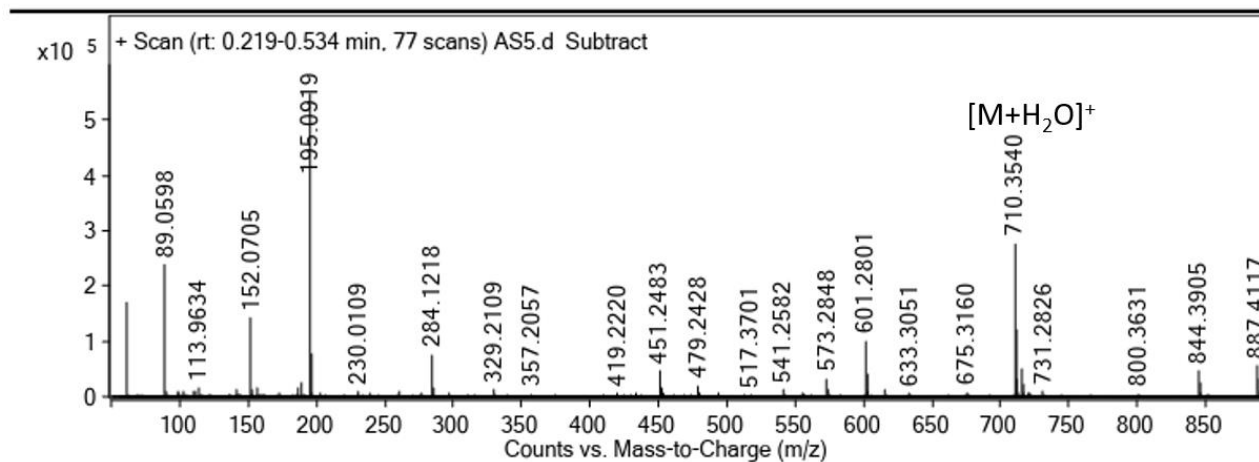


Figure S18. MS spectrum of compound **P2** (CDCl₃)

Qualitative Analysis Report



Peak List

m/z	z	Abund
61.0285	1	169672.11
89.0598	1	236870.75
152.0705	1	141642.3
188.9844		26439.52
195.0919	1	546454.56
196.0949	1	76147.08
284.1218	1	75256.98
451.2483	1	45962.73
573.2848	1	32360.98
601.2801	1	99619.84
602.2833	1	39579.84
710.354	1	275875.59
711.3573	1	119438.33
712.3597	1	31923.49
715.3092	1	48769.35
716.3123	1	20847.97
844.3905	1	45516.91
845.3935	1	24288.24
887.4117	1	55378.14
888.4146	1	32324.56

Figure S19. Structural novelty check of compound P2

The screenshot shows the CAS Scifinder search results for a drawn structure. The search criteria are set to "Substructure (2)" and "Similarity (155K)". Two results are displayed:

- 1946844-18-3**: C45H50O12. Absolute stereochemistry shown, Rotation (-). E/Z labels describe double bond geometry.
- 1946844-15-0**: C45H49BrO12. Benzoic acid, 4-bromo-, (1S,2R,3S,3a,5,4E,6R,8R,10E,12R,13R,13aR)-8,13a-bis(acety...).

Each result includes a chemical structure, a molecular formula, and buttons for "References", "Reactions", and "Supplier".

The summary panel shows the search criteria and options:

- Substances** 10:35 PM
- Chemical structure of the drawn structure.
- As Drawn (0)
- Substructure (2)
- Similarity (155K)
- Rerun Search** button
- Edit Search** button

Figure S20. ¹H-NMR (600 MHz, Acetone-*d*₆) spectrum of compound P3

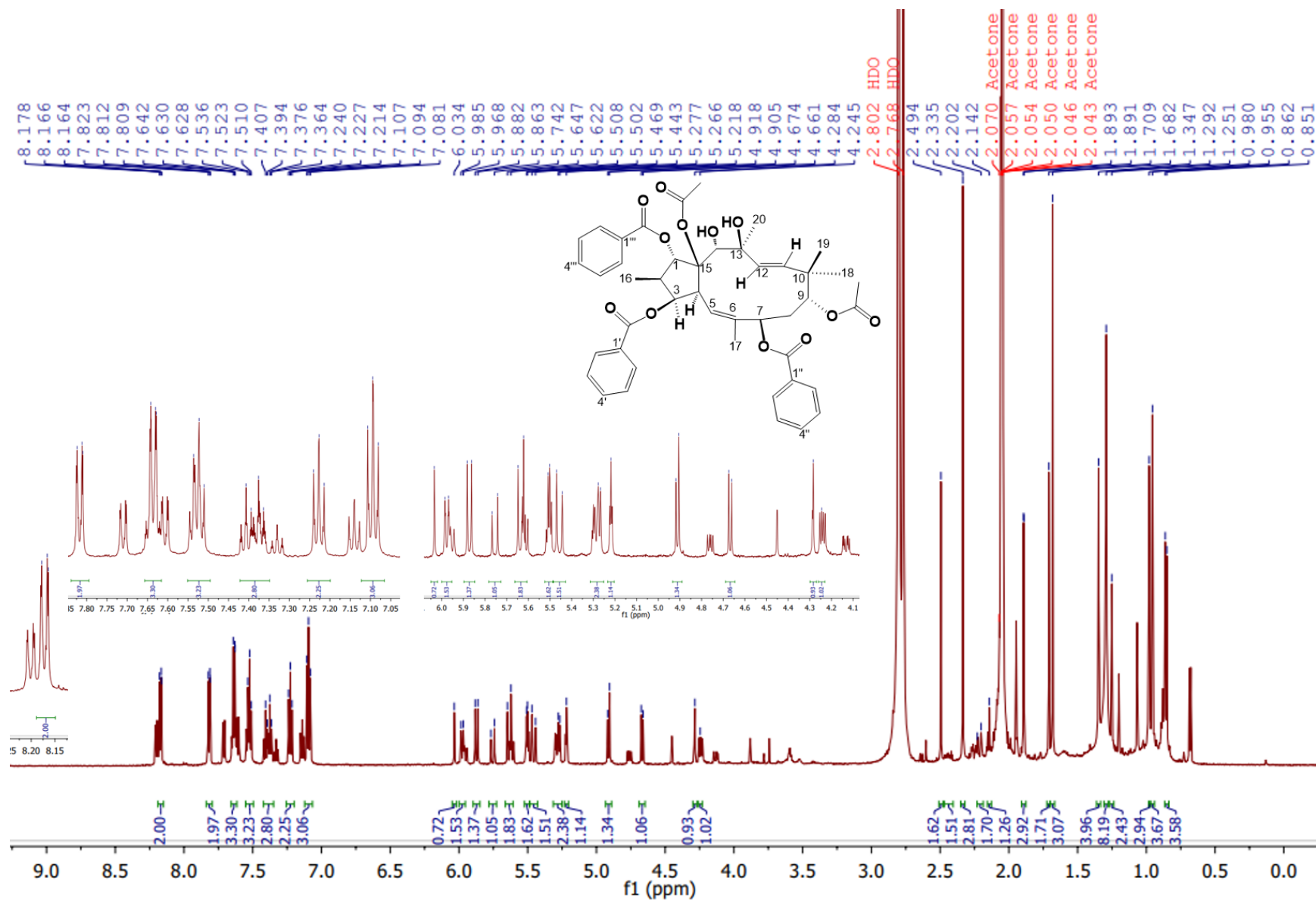


Figure S21. ¹H-NMR (600 MHz, Acetone-*d*₆) (sketched) spectrum of compound **P3**

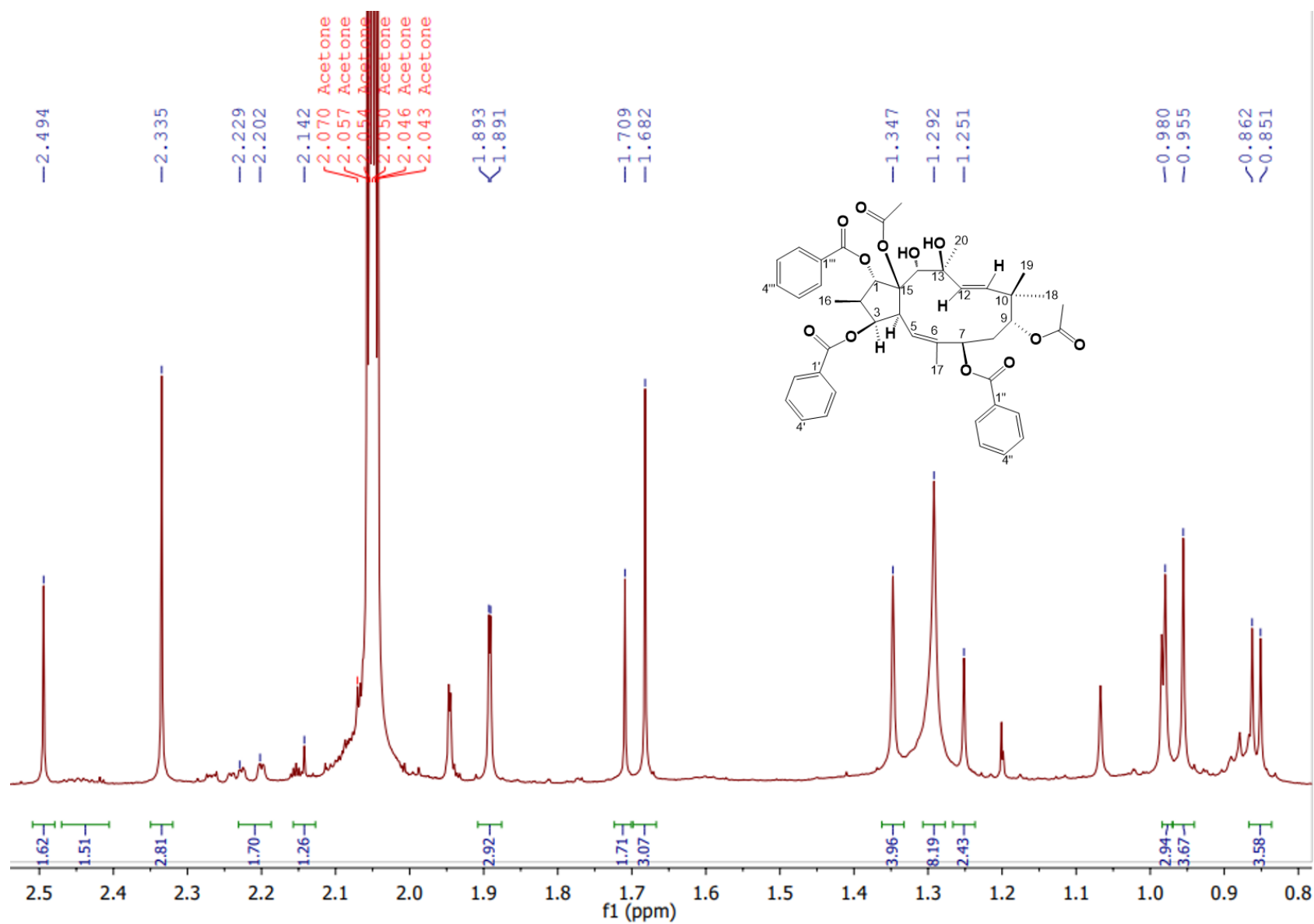


Figure S22. ^{13}C -NMR (125 MHz, Acetone- d_6) spectrum of compound P3

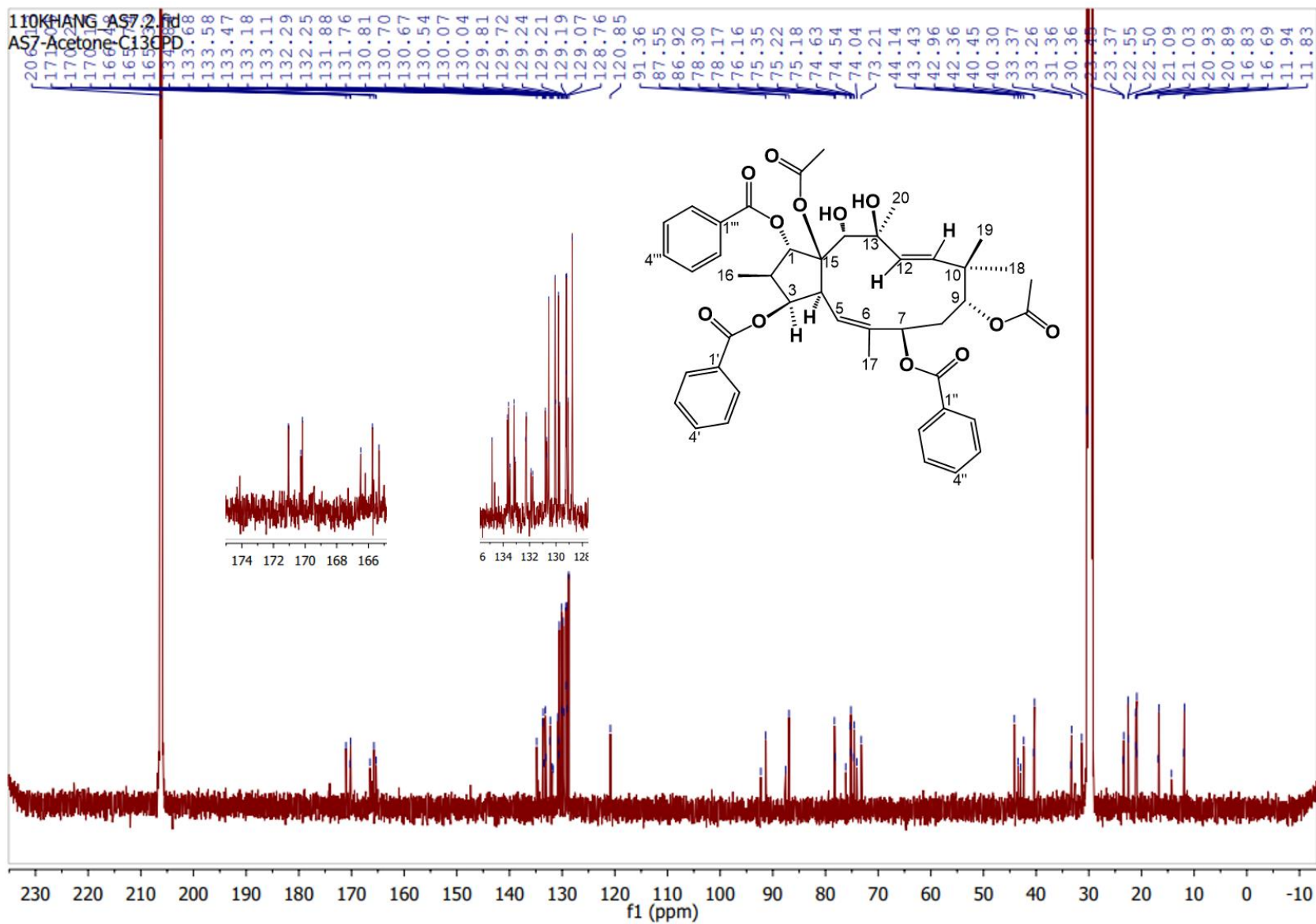


Figure S23. COSY spectrum of compound P3 (Acetone- d_6)

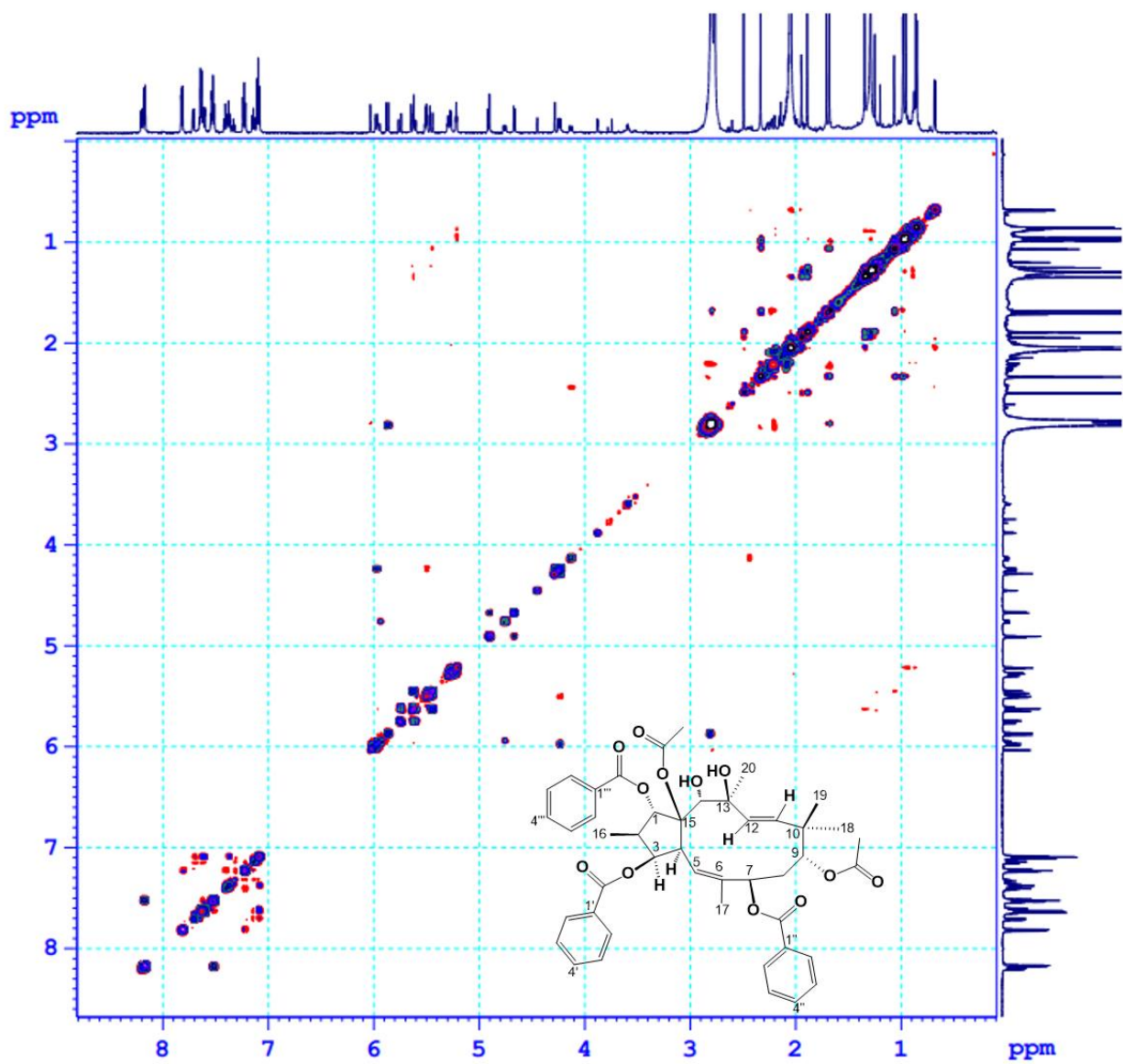


Figure S24. HSQC spectrum (total) of compound **P3** (Acetone- d_6)

AS07 HSQC

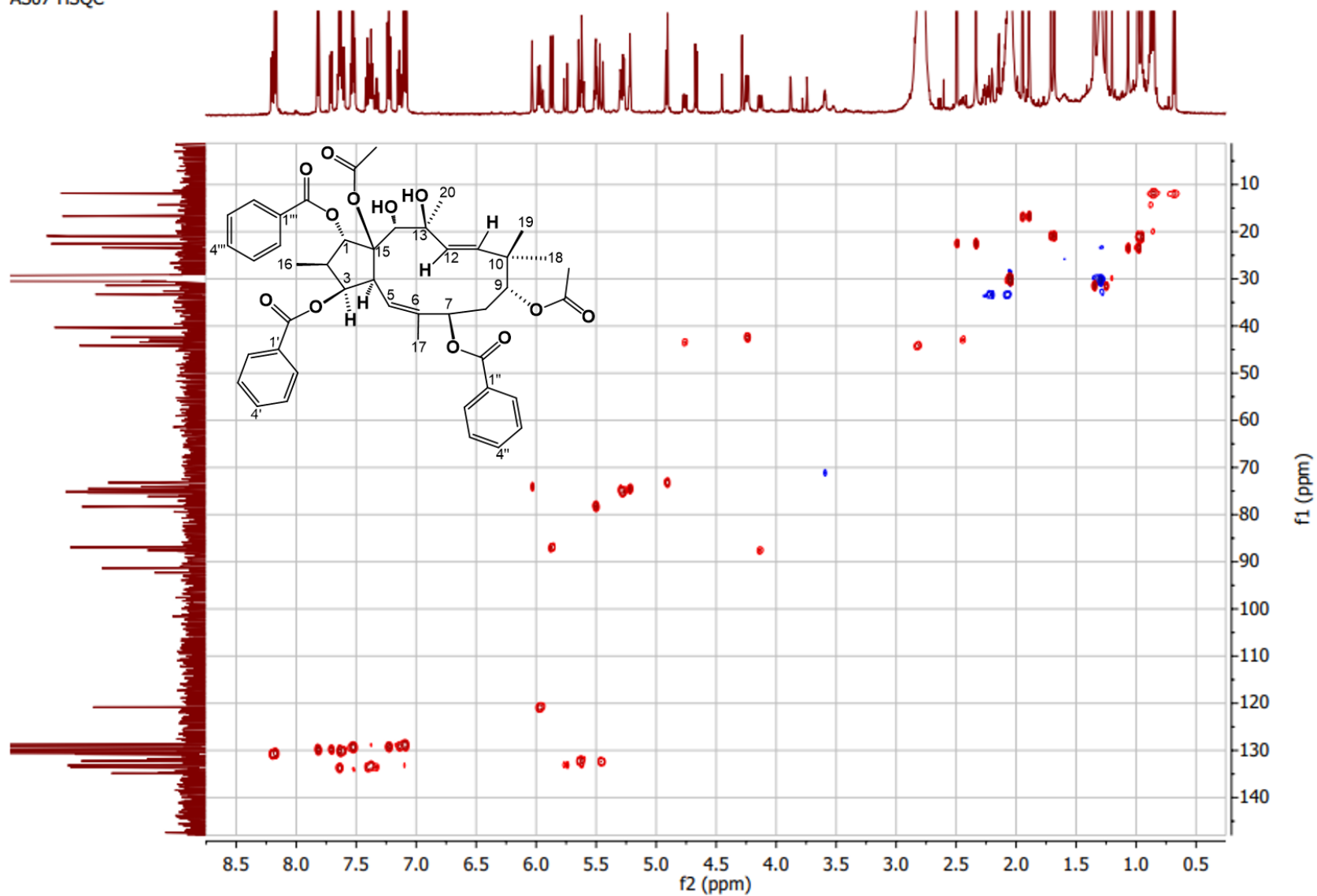


Figure S25. HSQC spectrum (sketched) of compound **P3** (Acetone- d_6)

AS07 HSQC

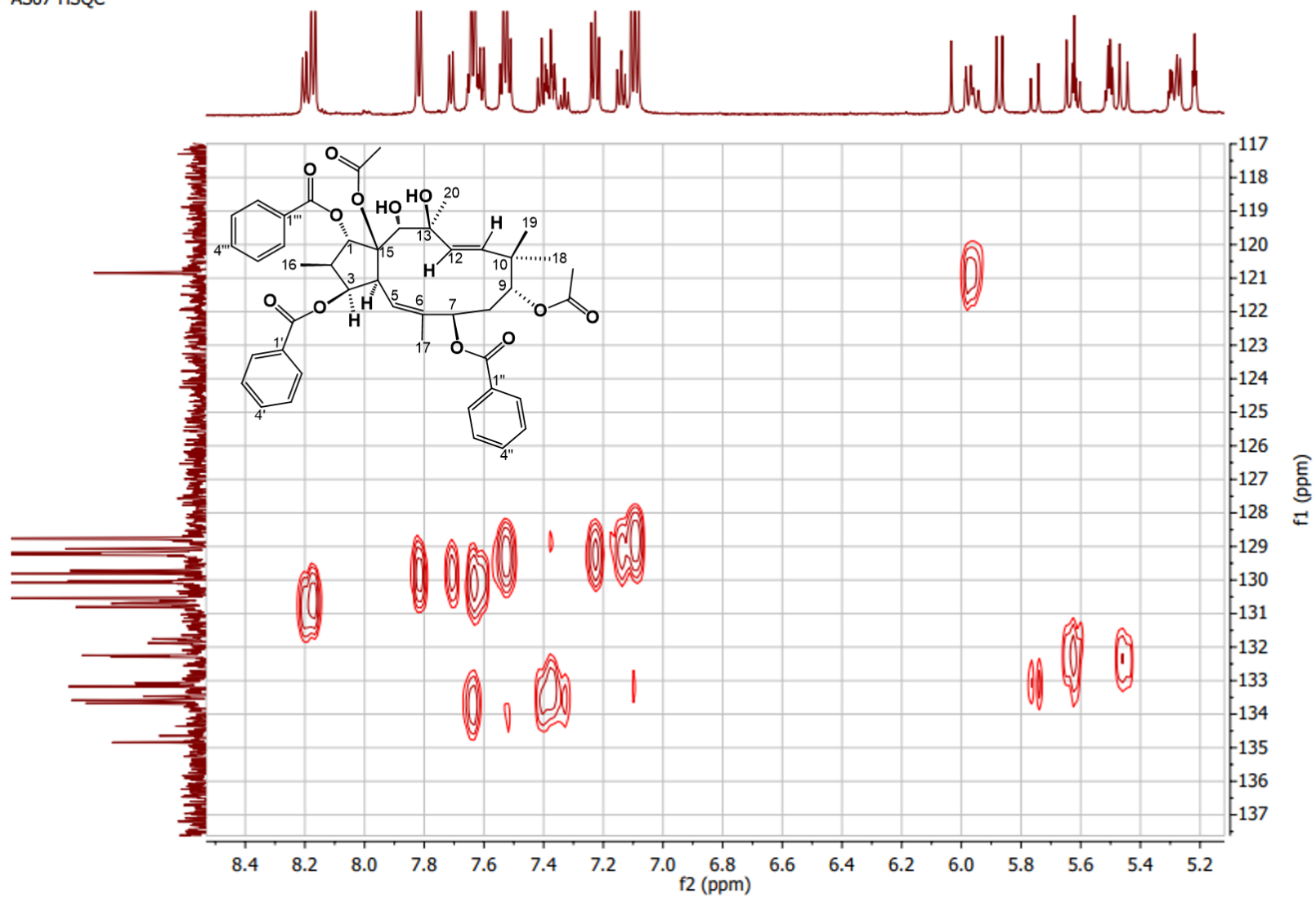


Figure S26. HMBC spectrum (total) of compound **P3** (Acetone- d_6)

AS07 HMBC

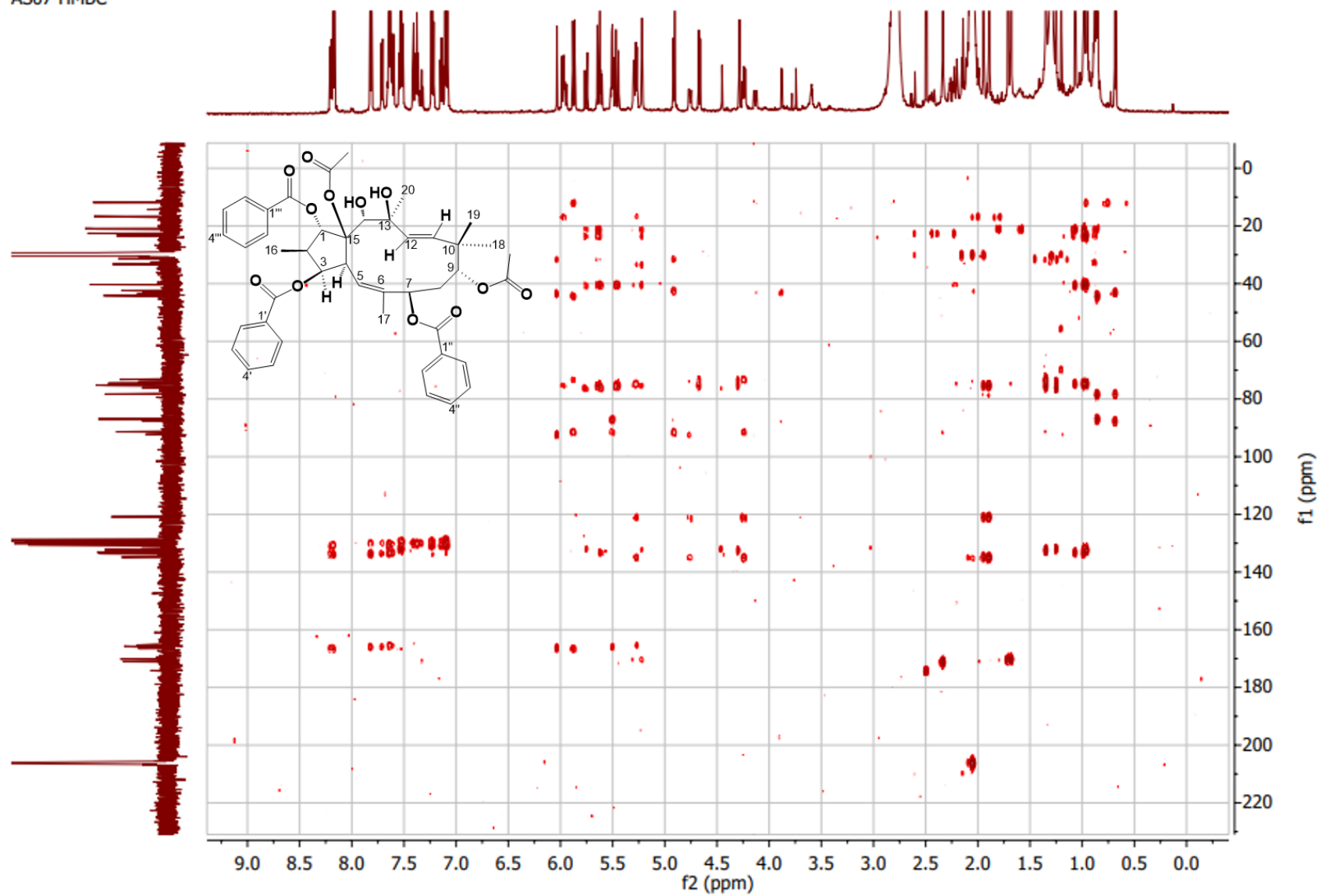


Figure S27. HMBC spectrum (sketched) of compound P3 (Acetone- d_6)

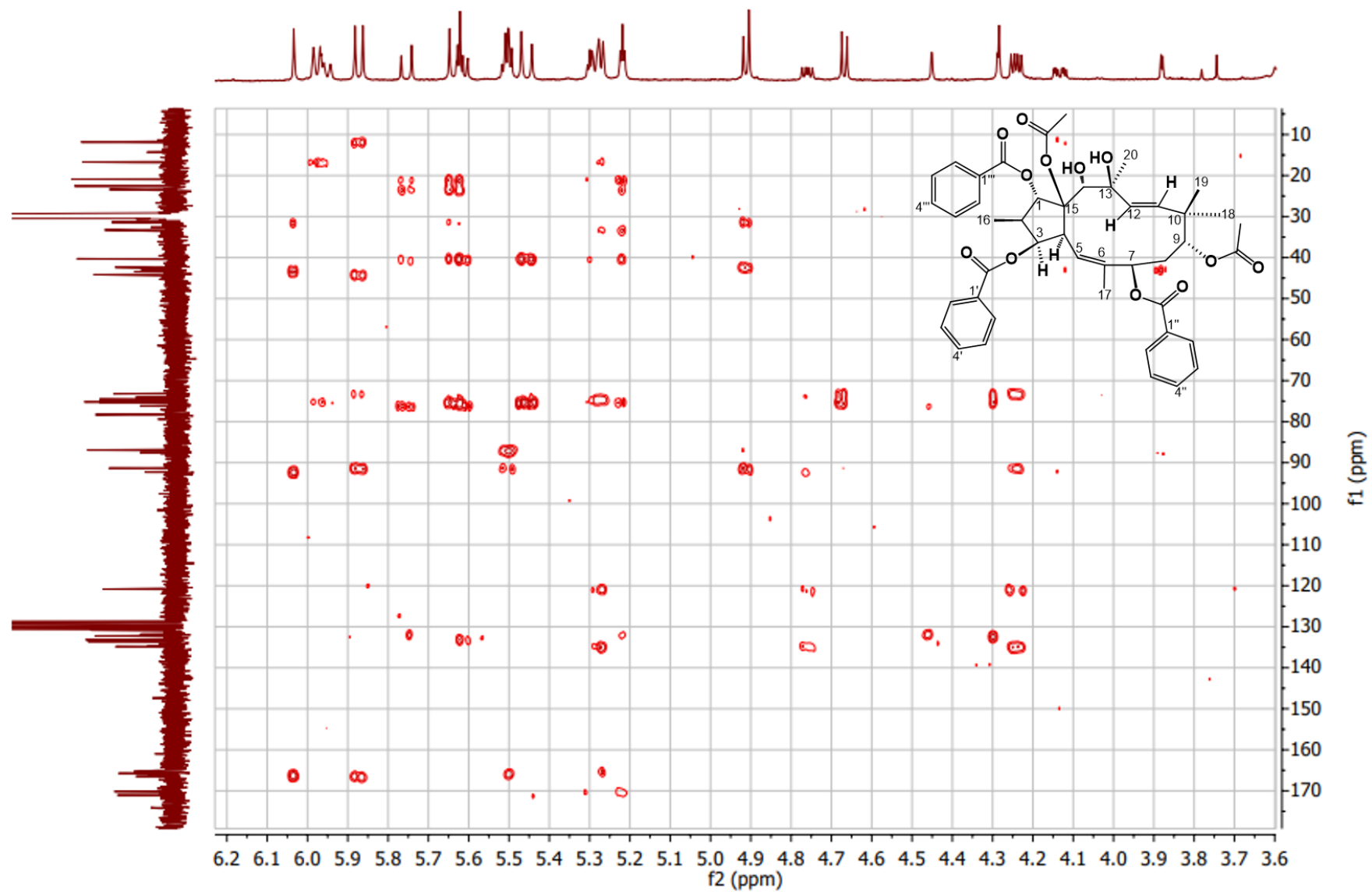


Figure S28. HMBC spectrum (sketched) of compound P3 (Acetone- d_6)

AS07 HMBC

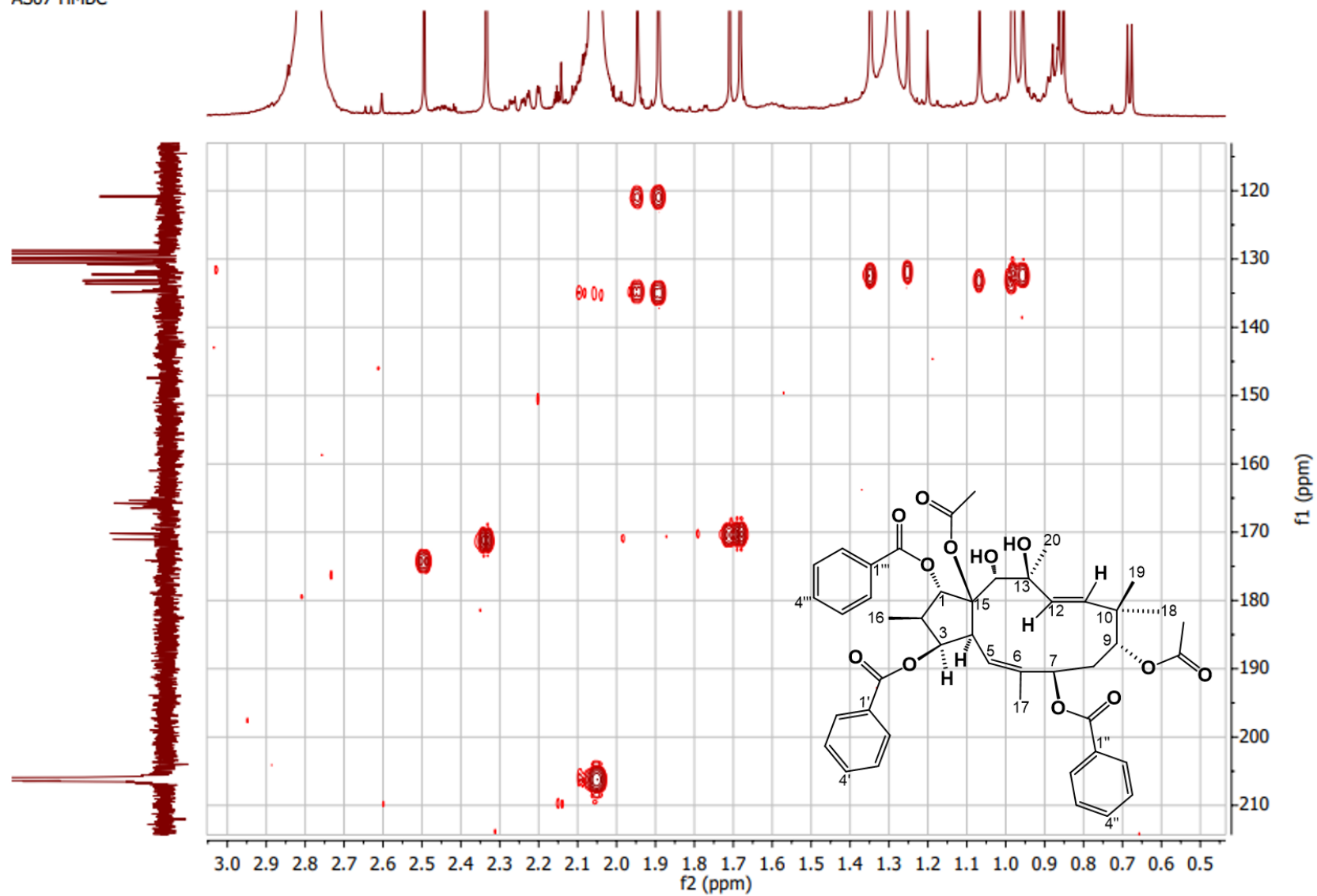


Figure S29. HMBC spectrum (sketched) of compound P3 (Acetone- d_6)

AS07 HMBC

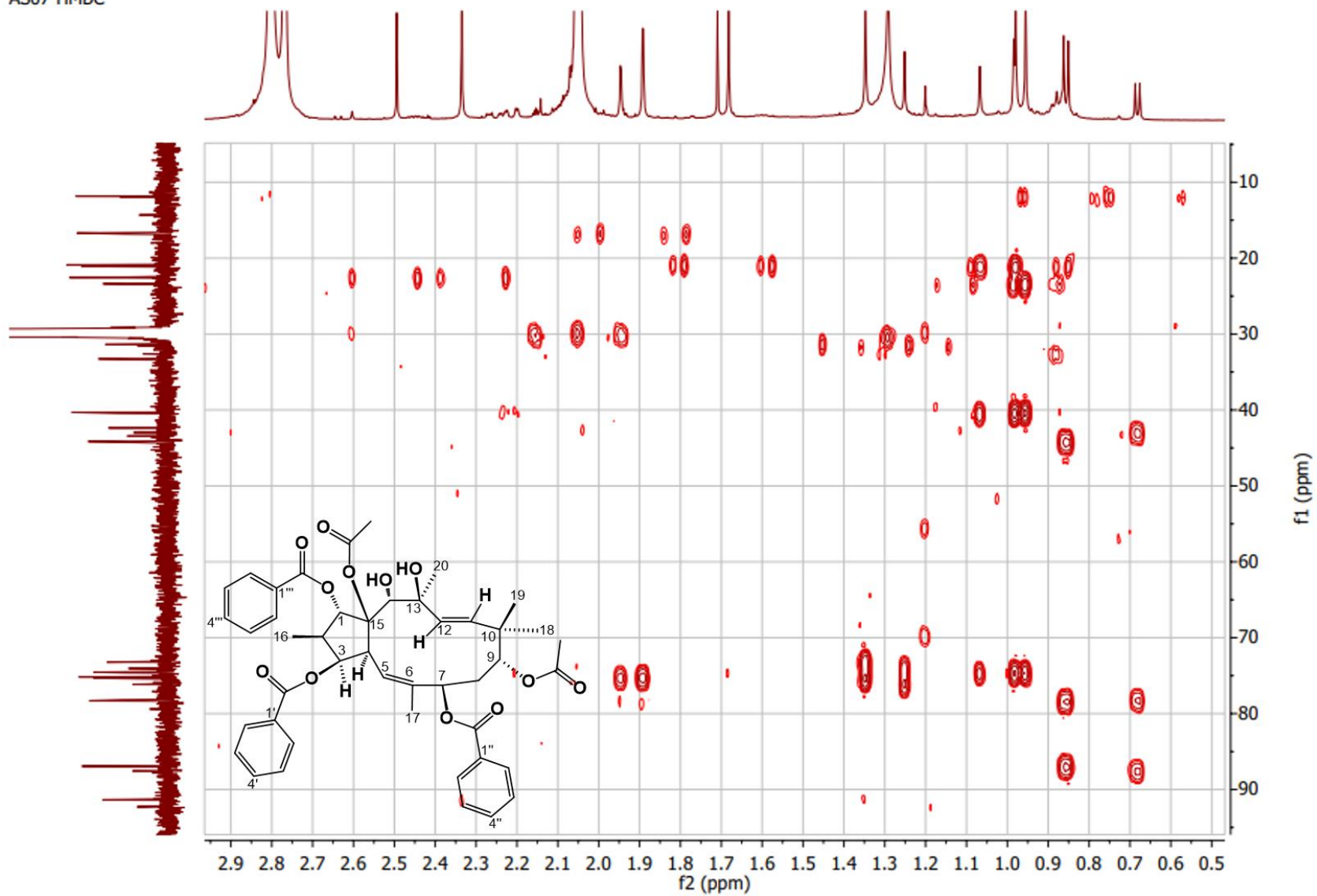


Figure S30. NOESY spectrum of compound **P3** (Acetone- d_6)

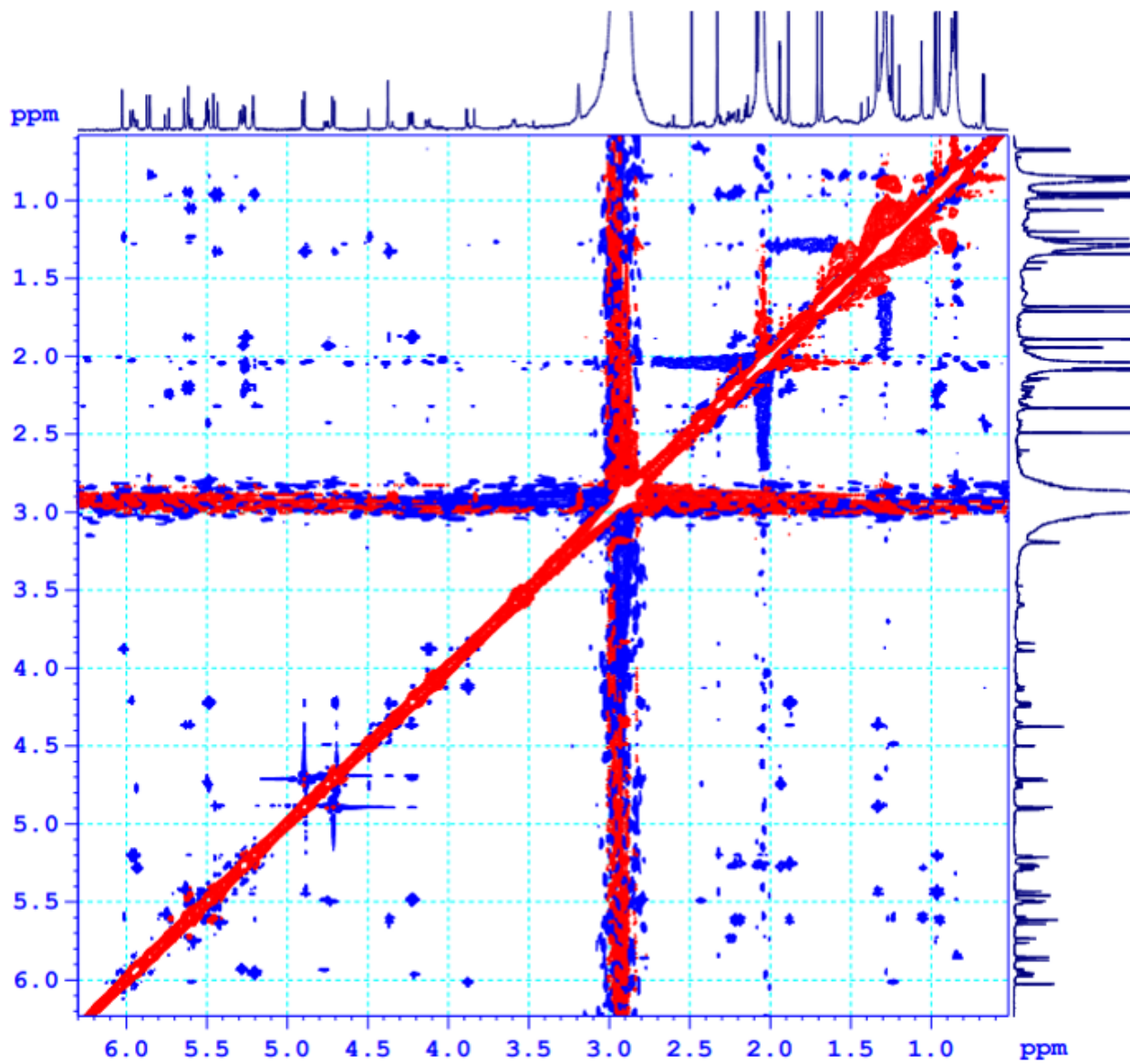


Figure S31. NOESY spectrum (sketched) of compound P3 (Acetone- d_6)

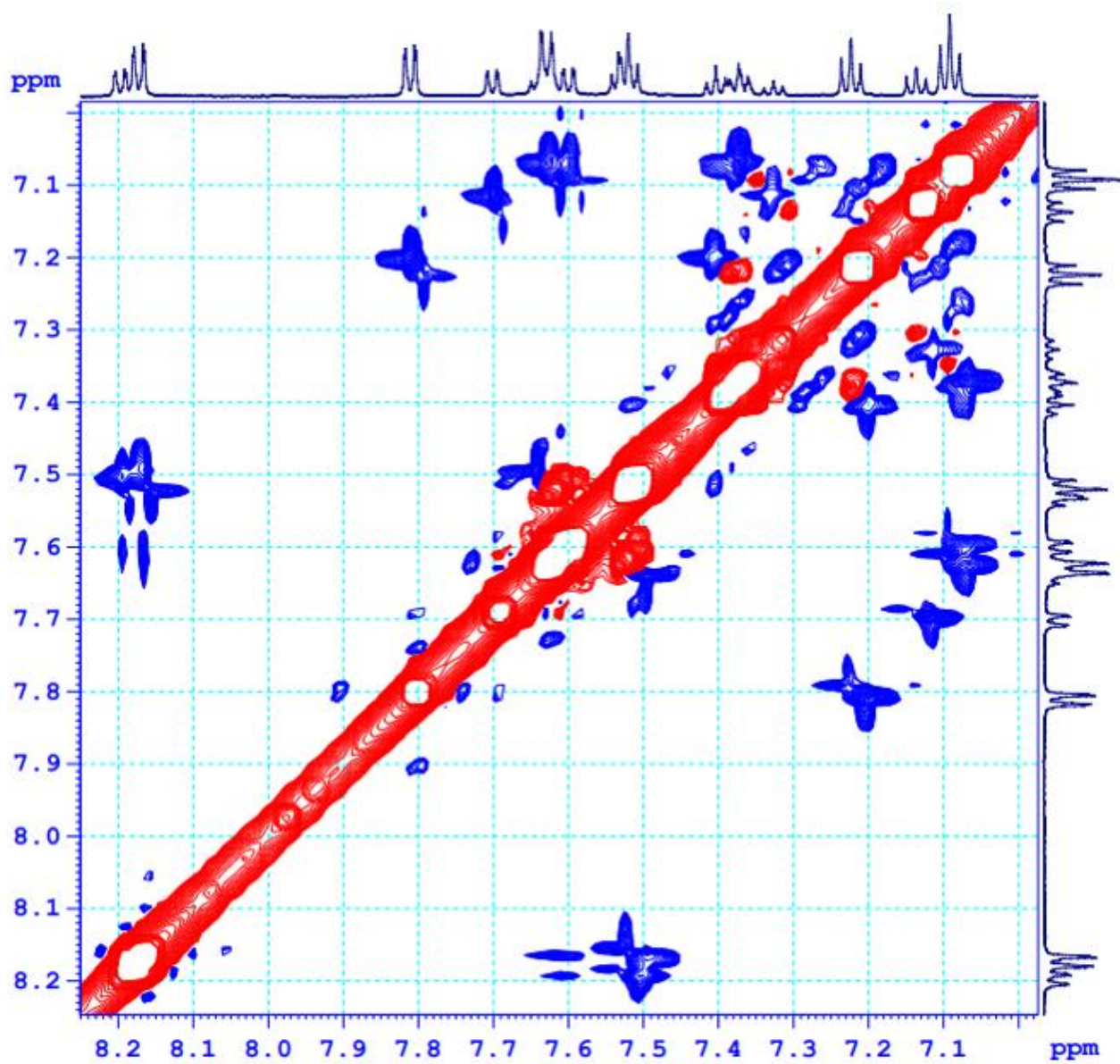


Figure S32. NOESY spectrum (sketched) of compound P3 (Acetone- d_6)

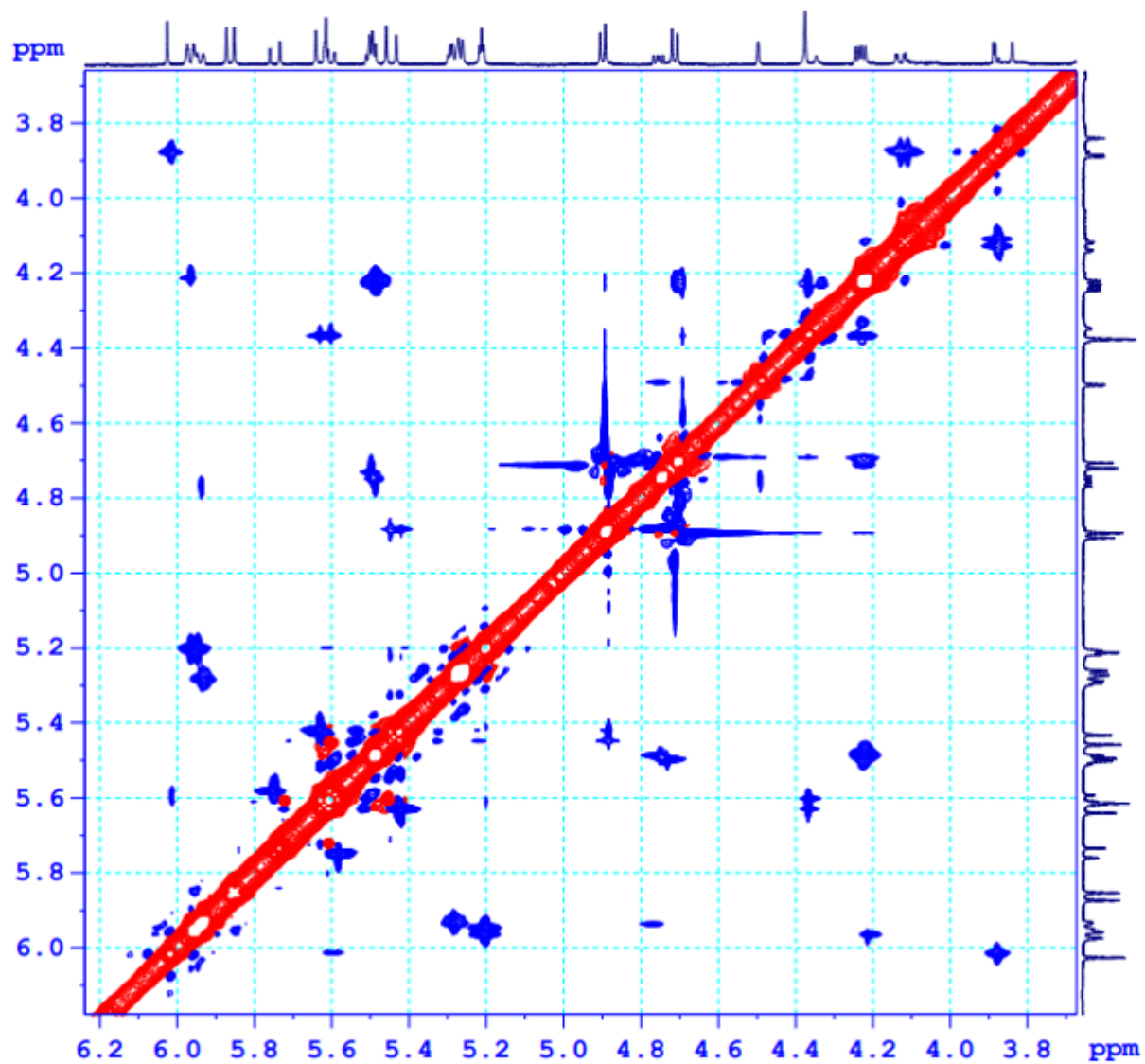


Figure S33. MS spectrum of compound **P3** (Acetone- d_6)

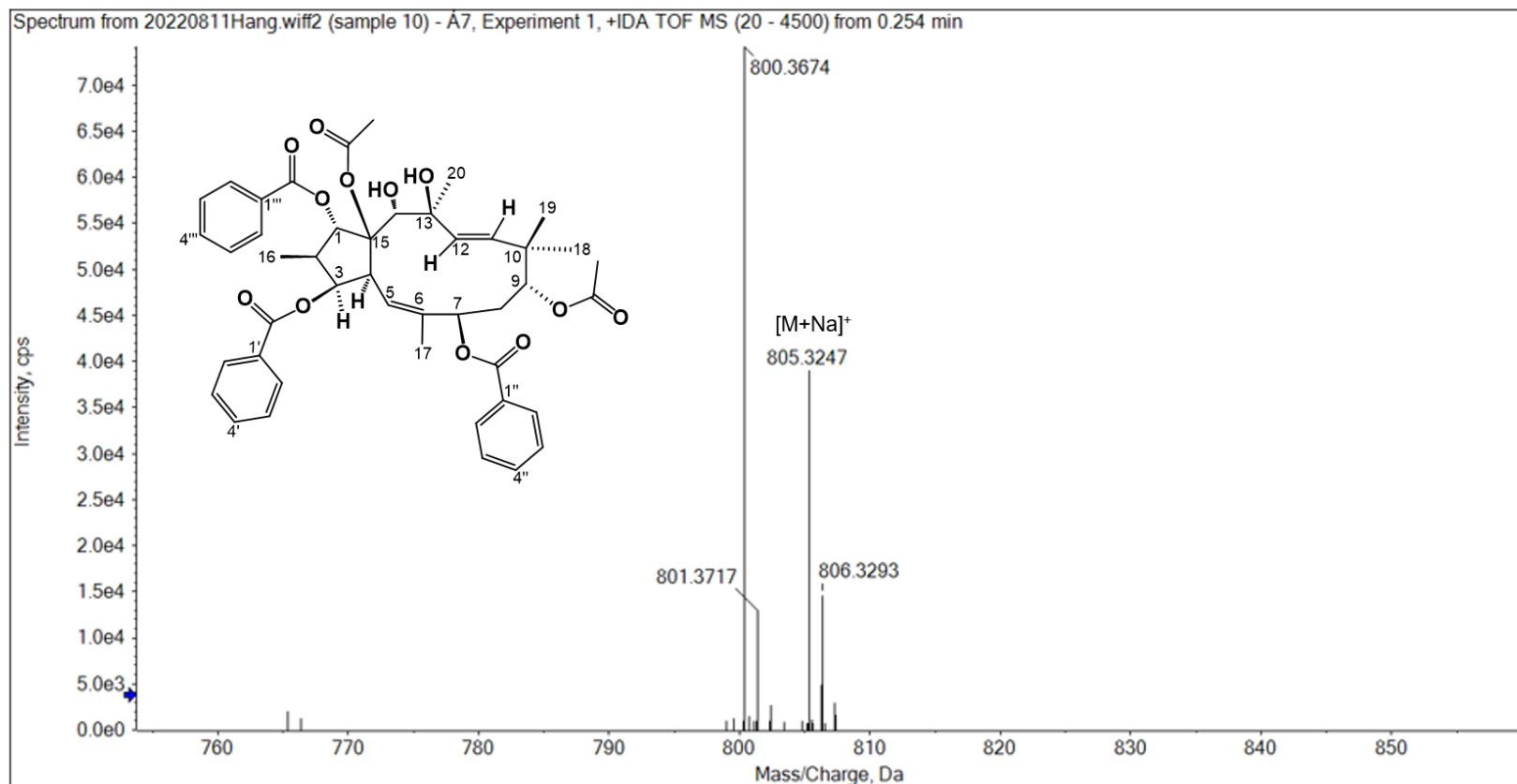


Figure S34. ¹H-NMR (600 MHz) spectrum of compound P4 (CDCl₃)

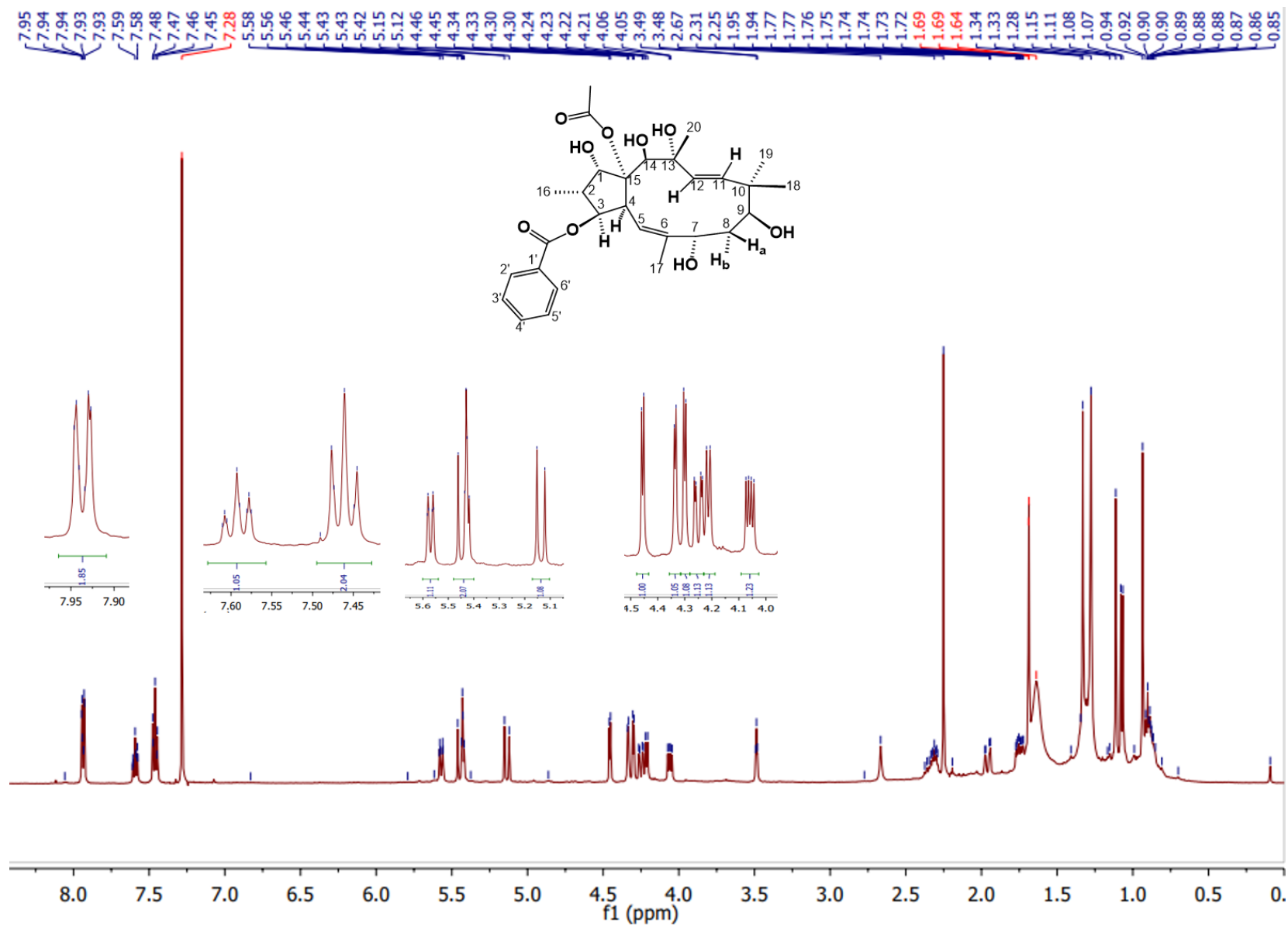


Figure S35. ^{13}C -NMR (125 MHz) spectrum of compound **P4** (CDCl_3)

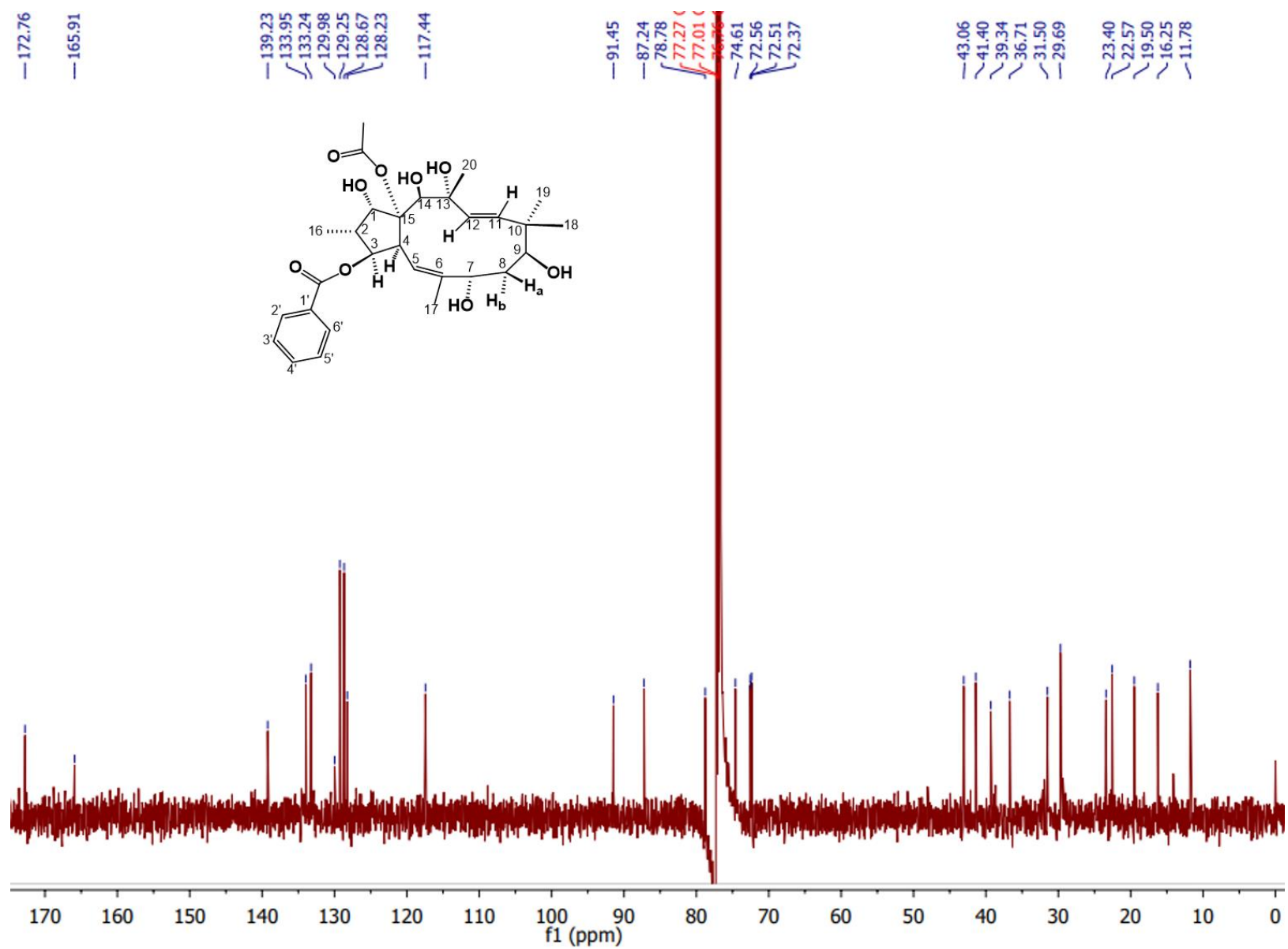


Figure S36. COSY spectrum of compound P4 (CDCl₃)

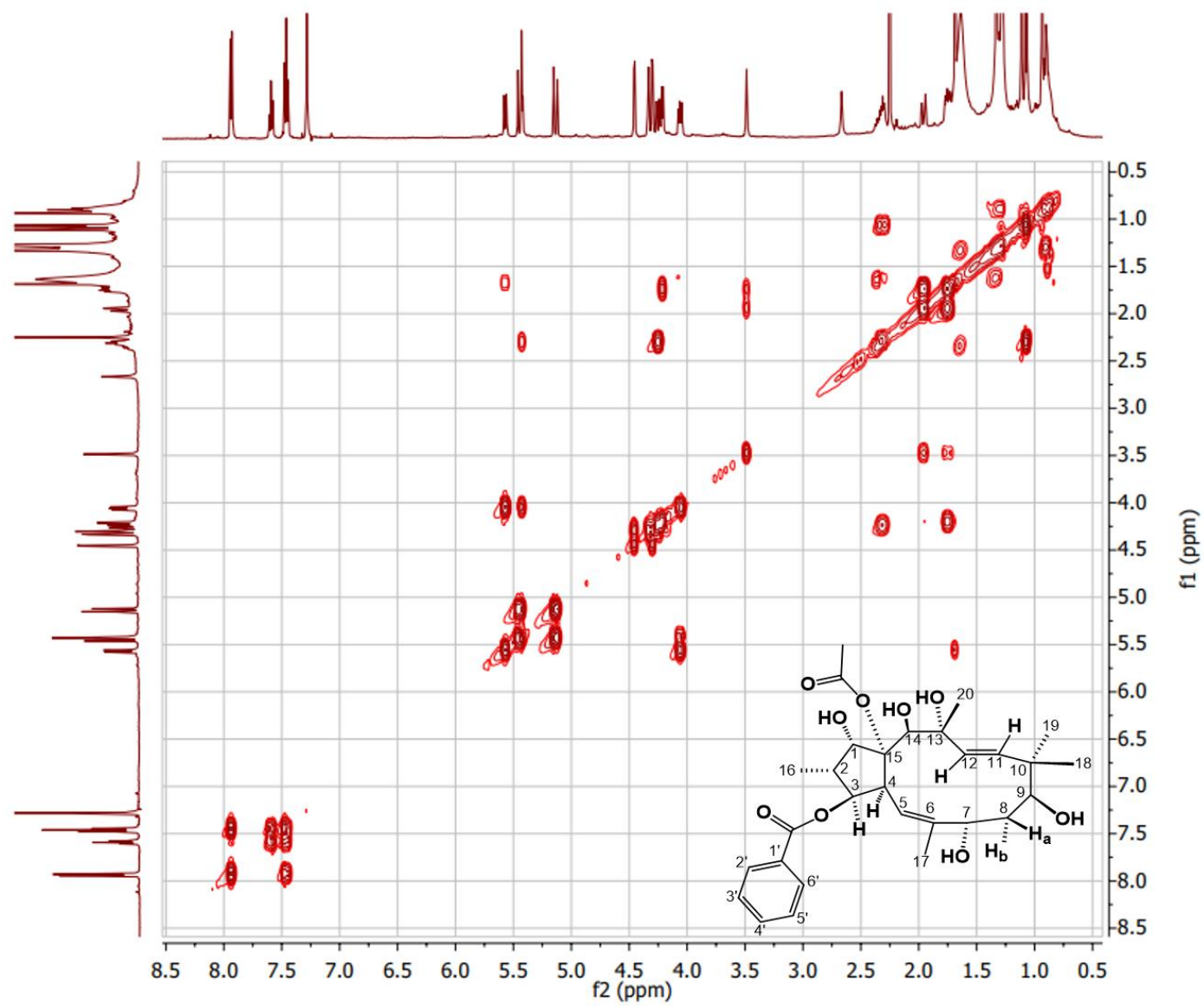


Figure S37. HSQC spectrum of compound P4 (CDCl₃)

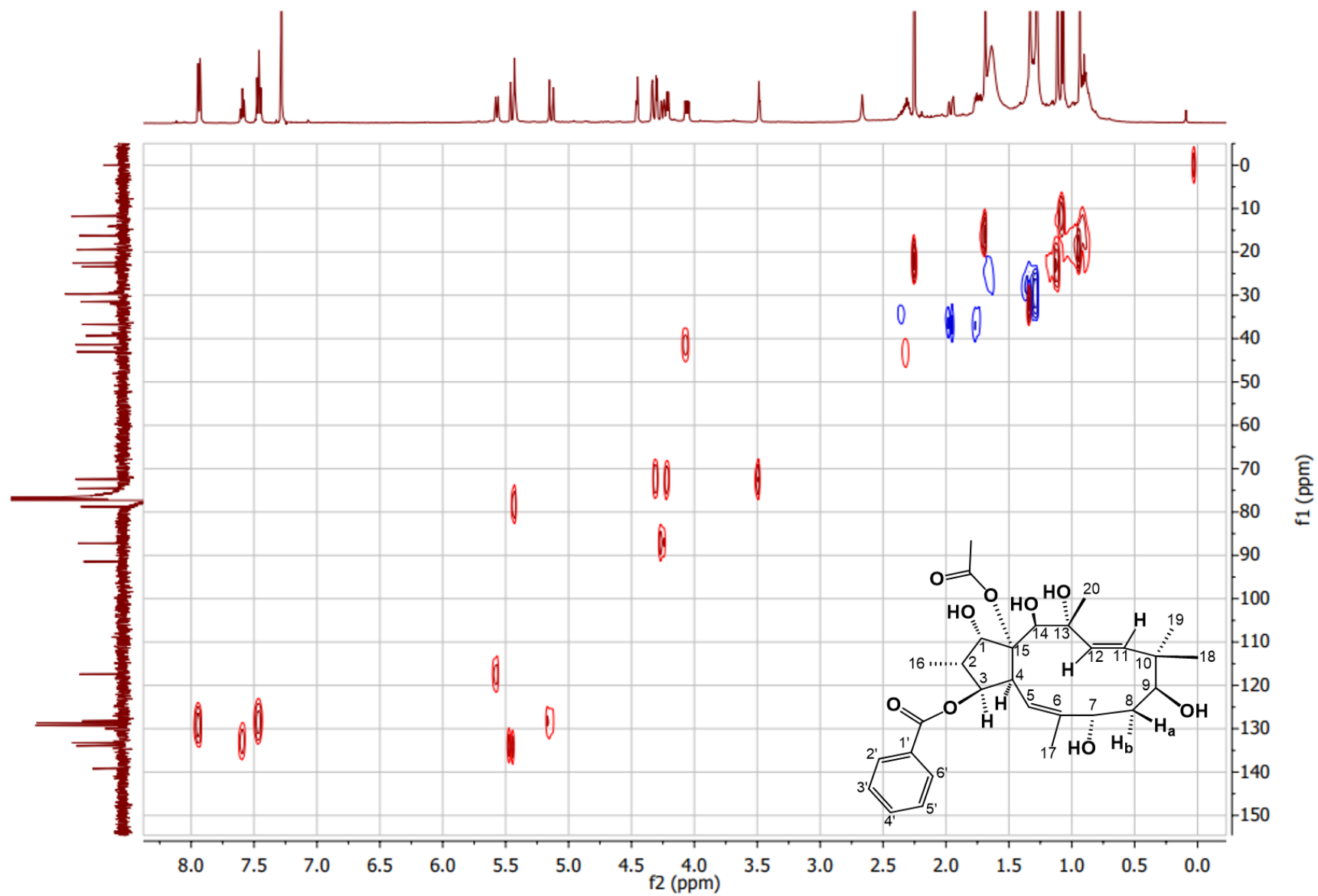


Figure S38. HMBC spectrum (total) of compound **P4** (CDCl₃)

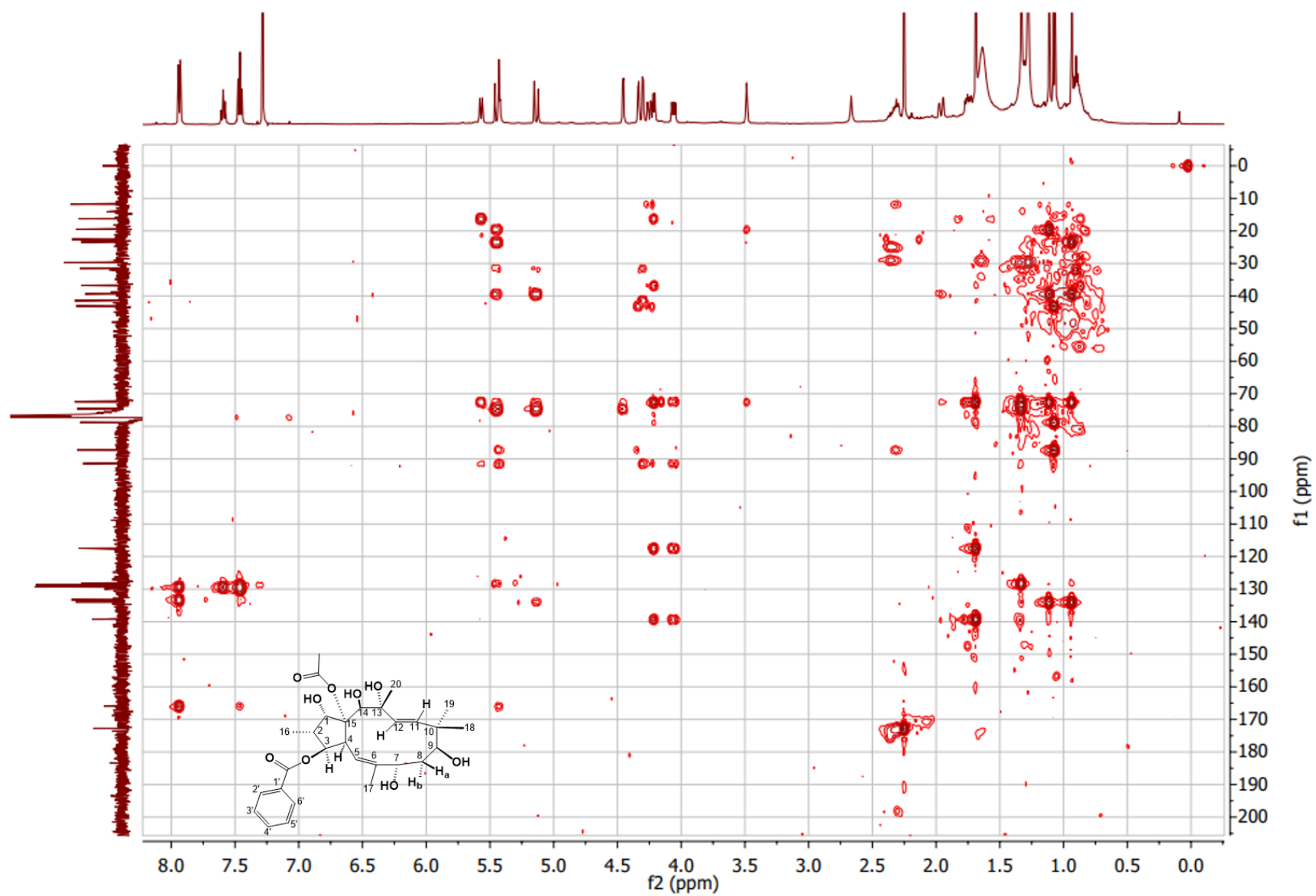


Figure S39. HMBC spectrum (sketched) of compound P4 (CDCl₃)

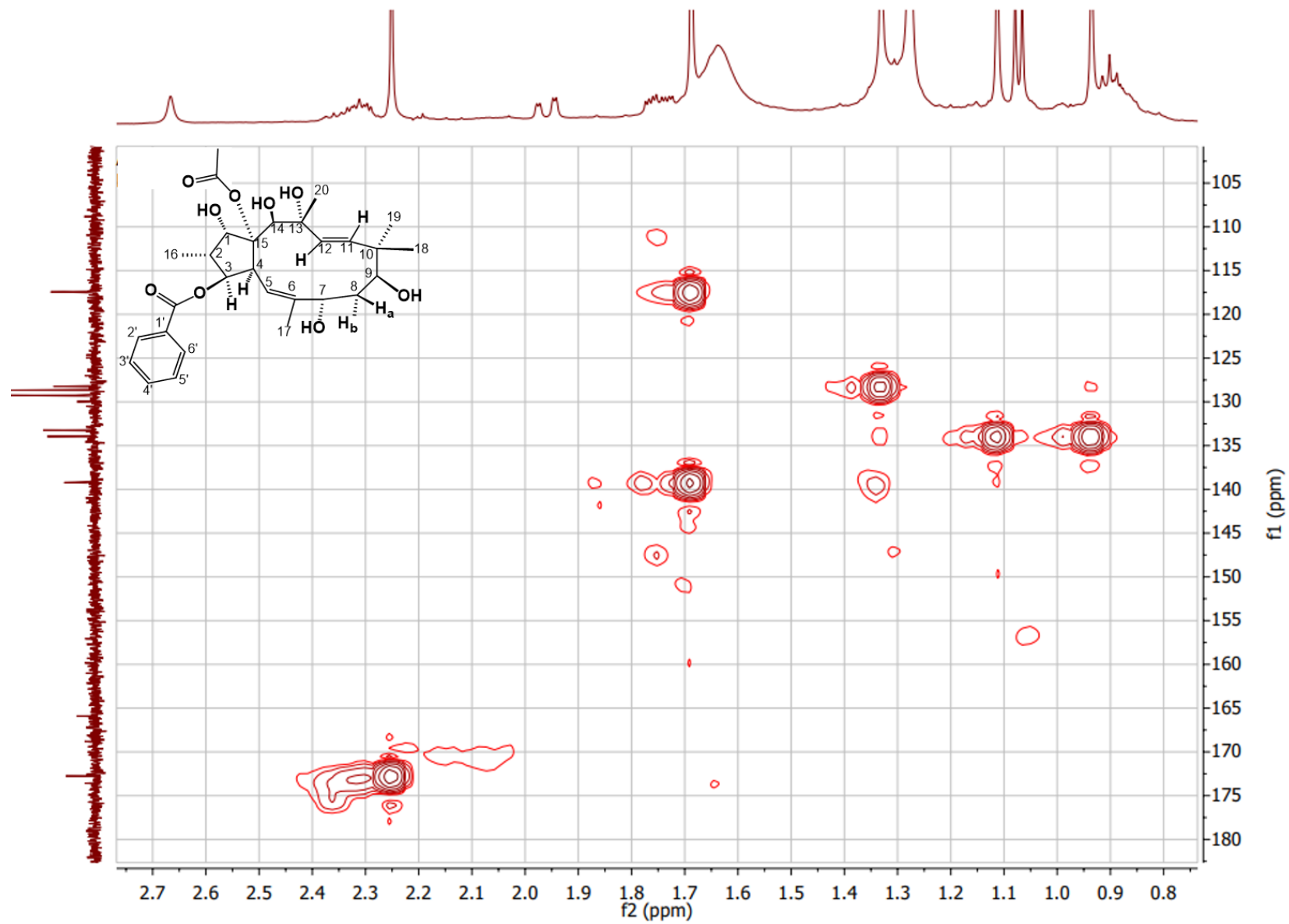


Figure S40. NOESY spectrum of compound **P4** (CDCl₃)

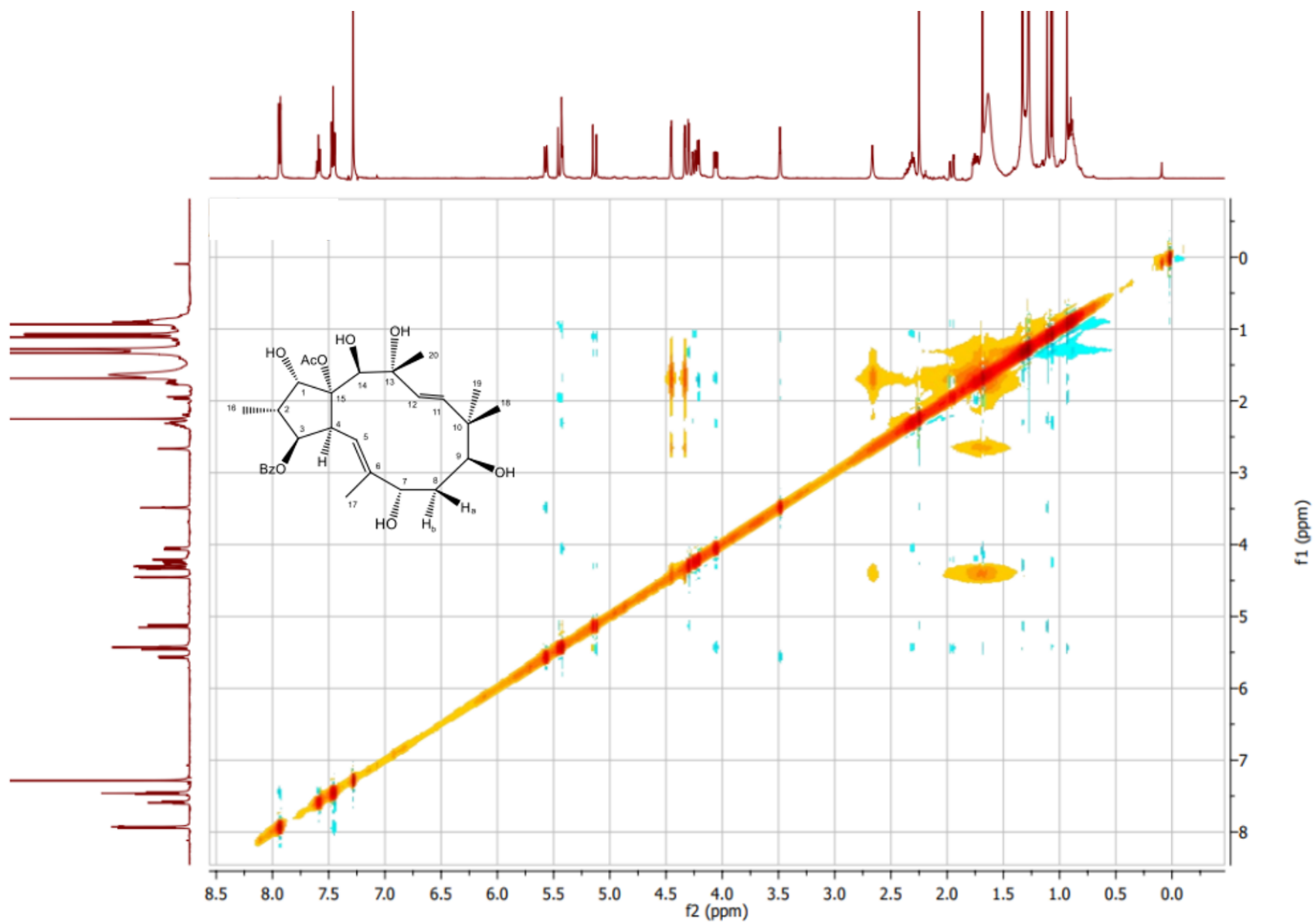
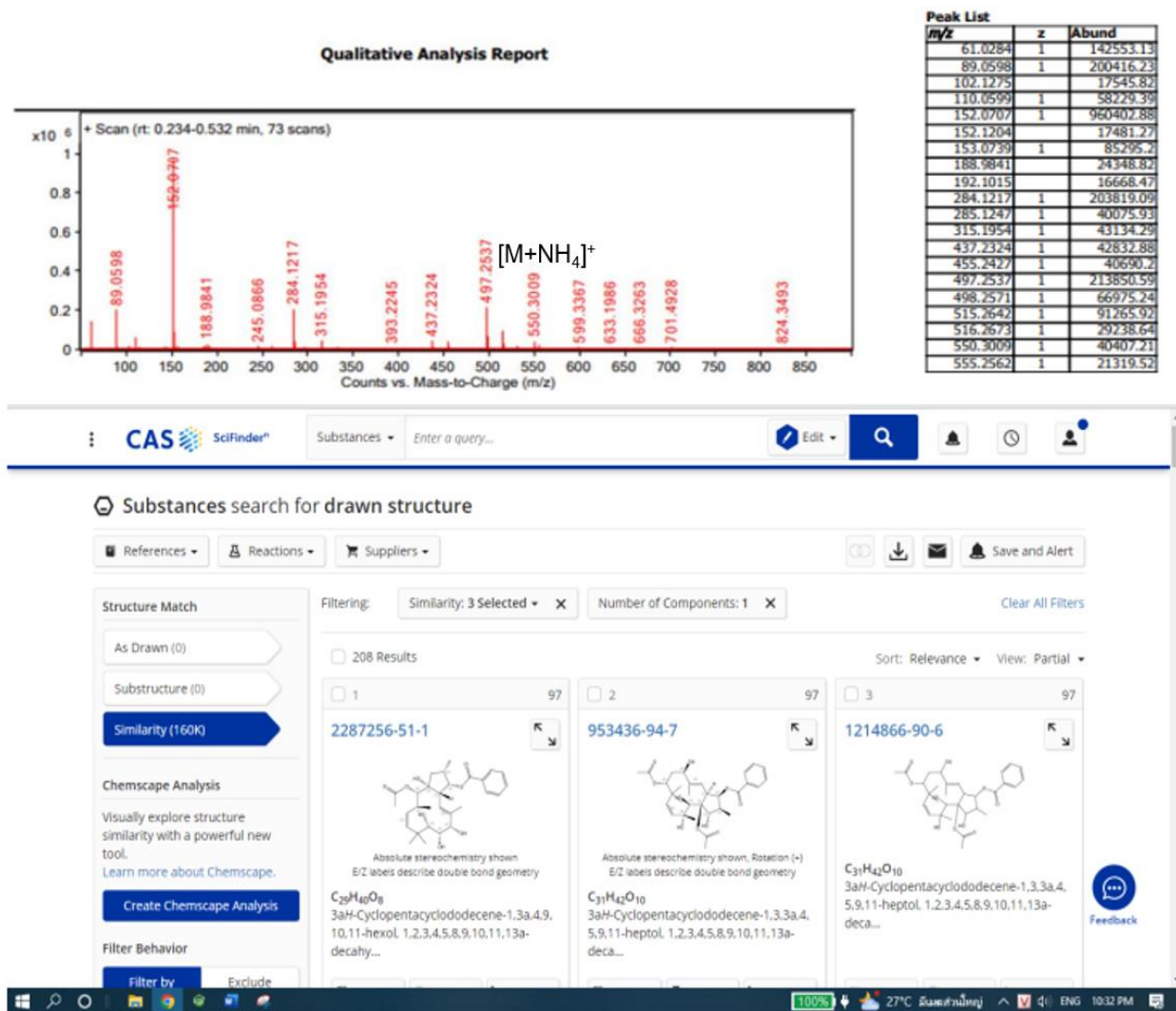


Figure S41. MS spectrum (CDCl₃) and structural novelty check for compound P4



Substances
10:31 PM

As Drawn (0)
Substructure (0)
Similarity (160K)

Rerun Search
Edit Search

Figure S42. ¹H-NMR (600 MHz) spectrum of compound P5 (CDCl₃)

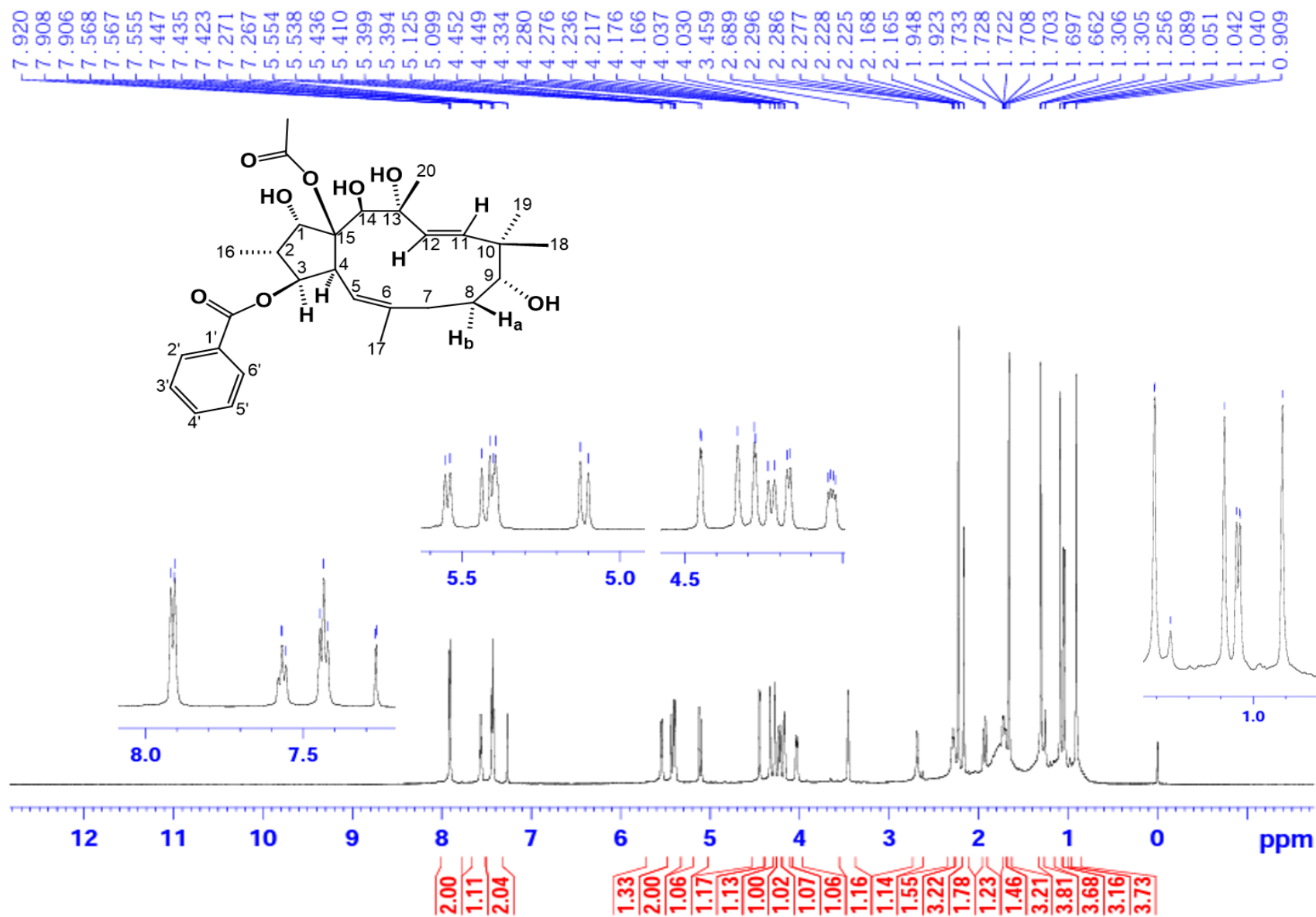


Figure S43. ^{13}C -NMR (125 MHz) spectrum of compound **P5** (CDCl_3)

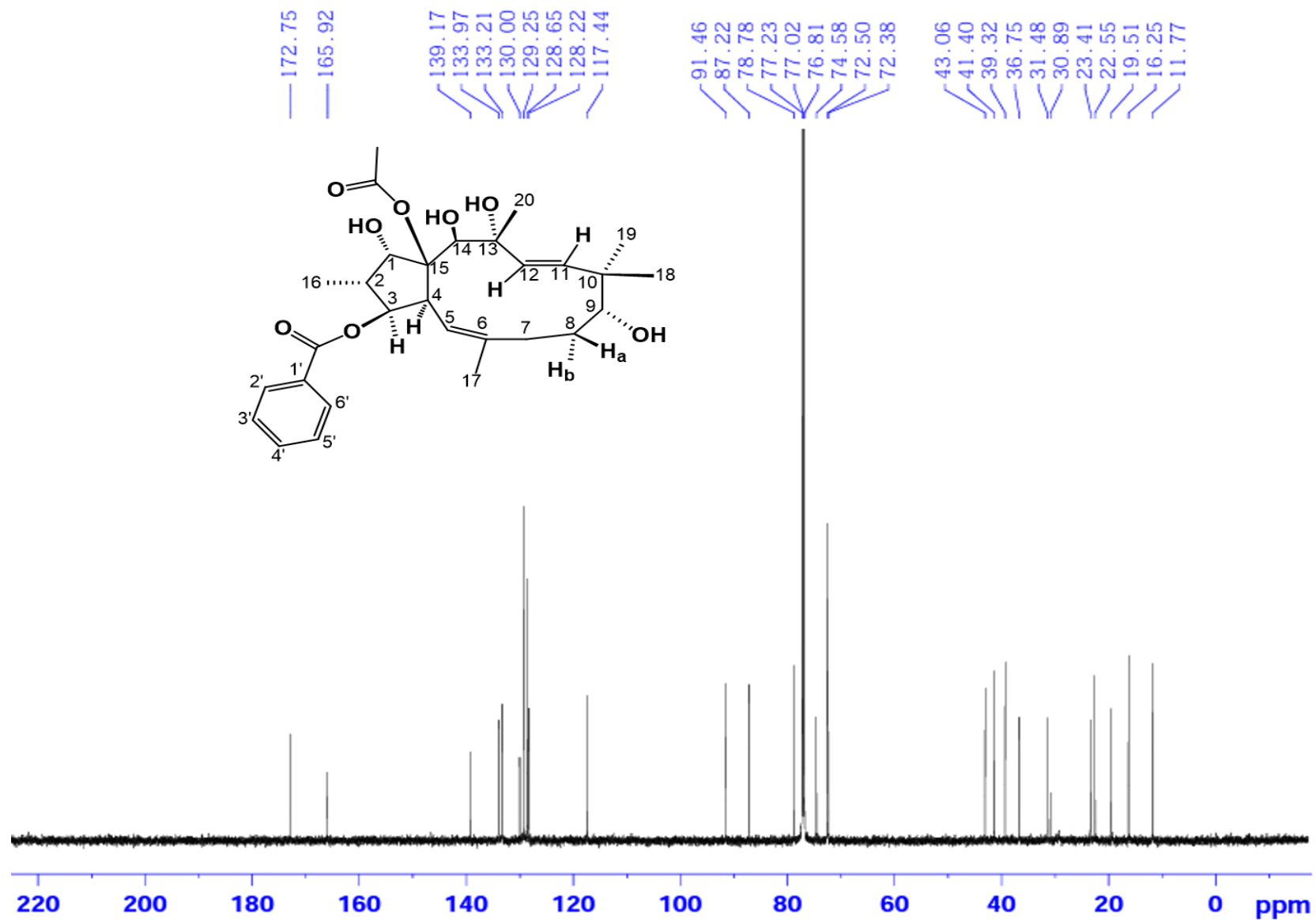


Figure S44. COSY spectrum of compound P5 (CDCl₃)

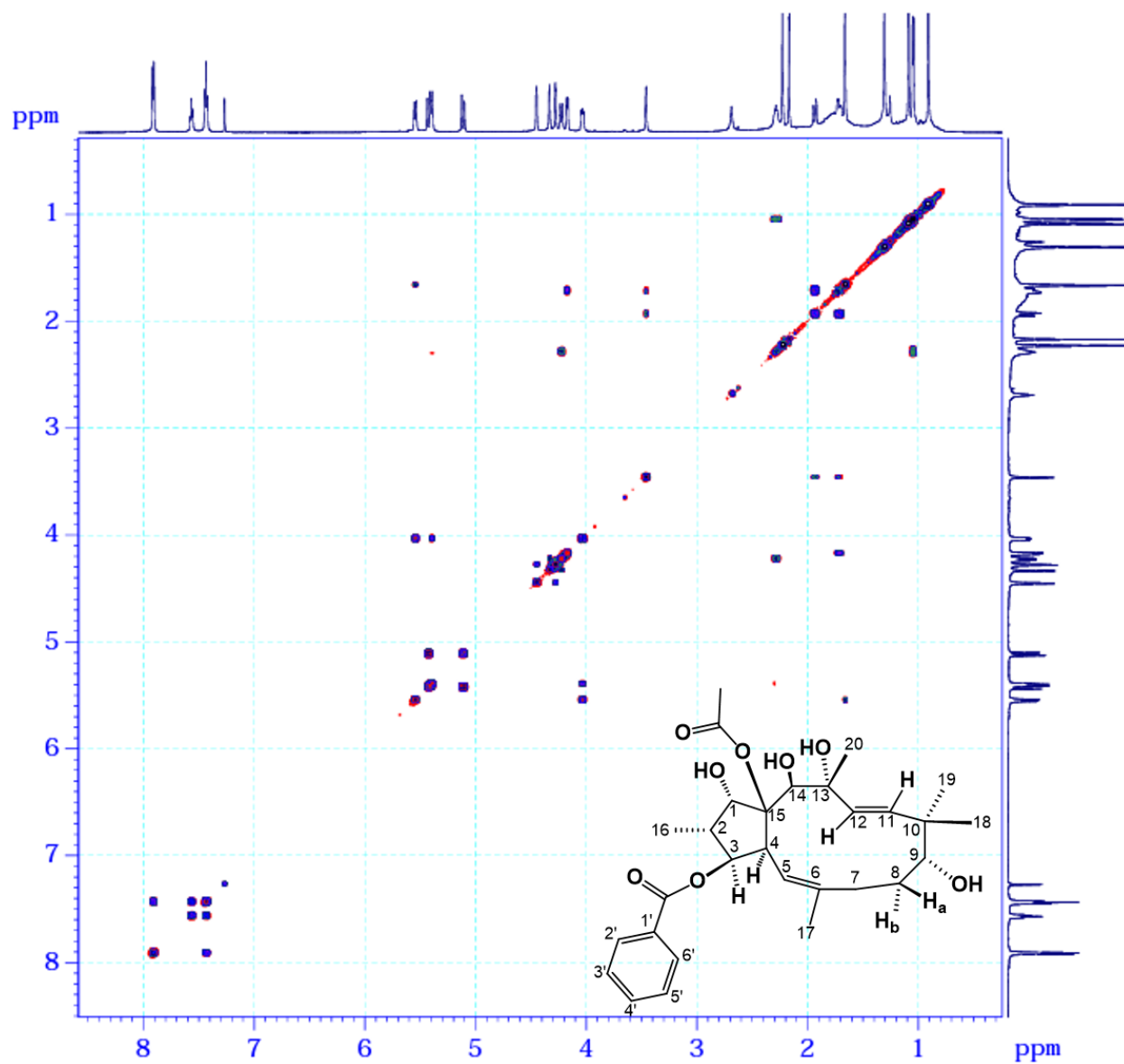


Figure S45. HSQC spectrum of compound P5 (CDCl₃)

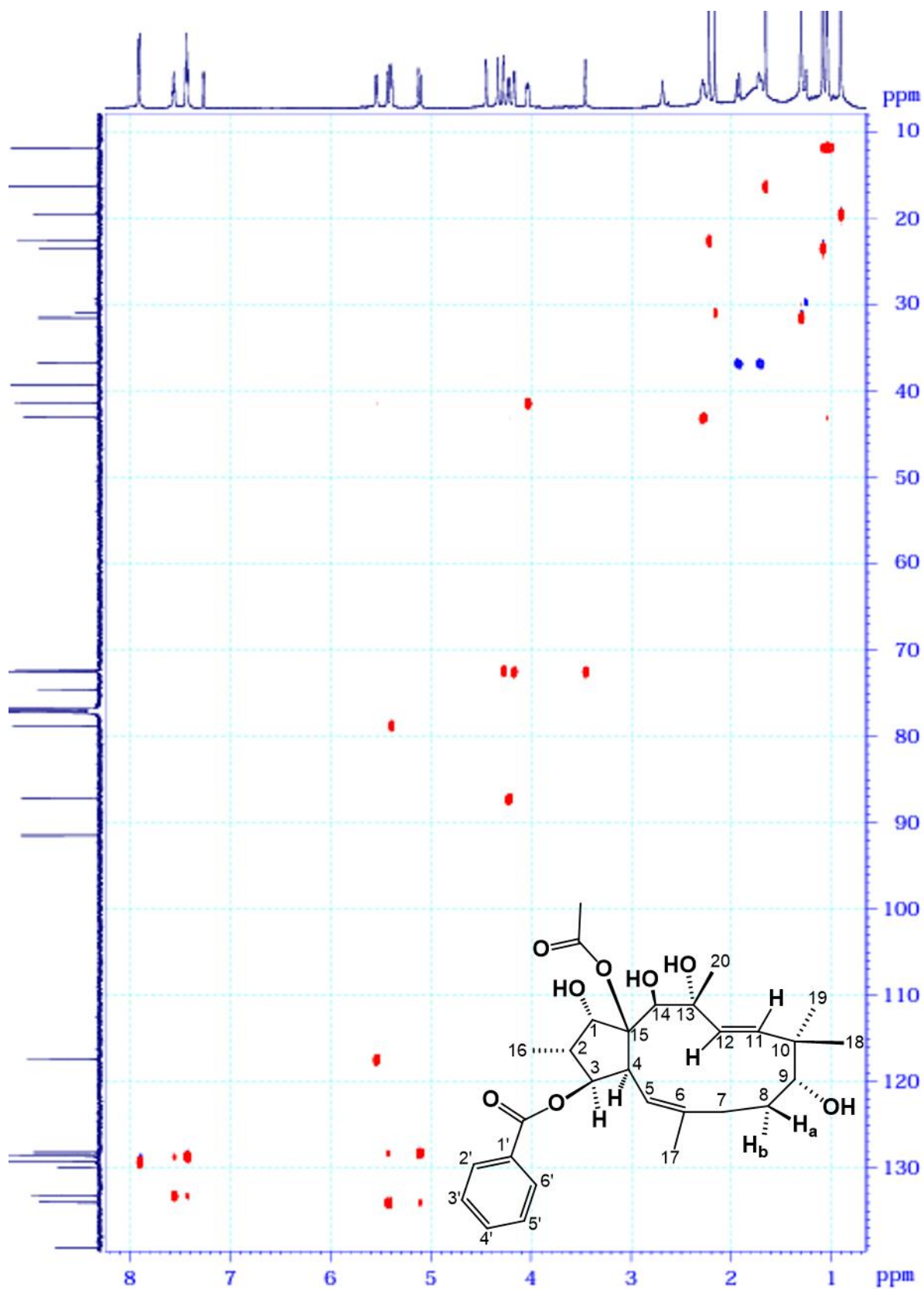


Figure S46. HMBC spectrum (total) of compound P5 (CDCl₃)

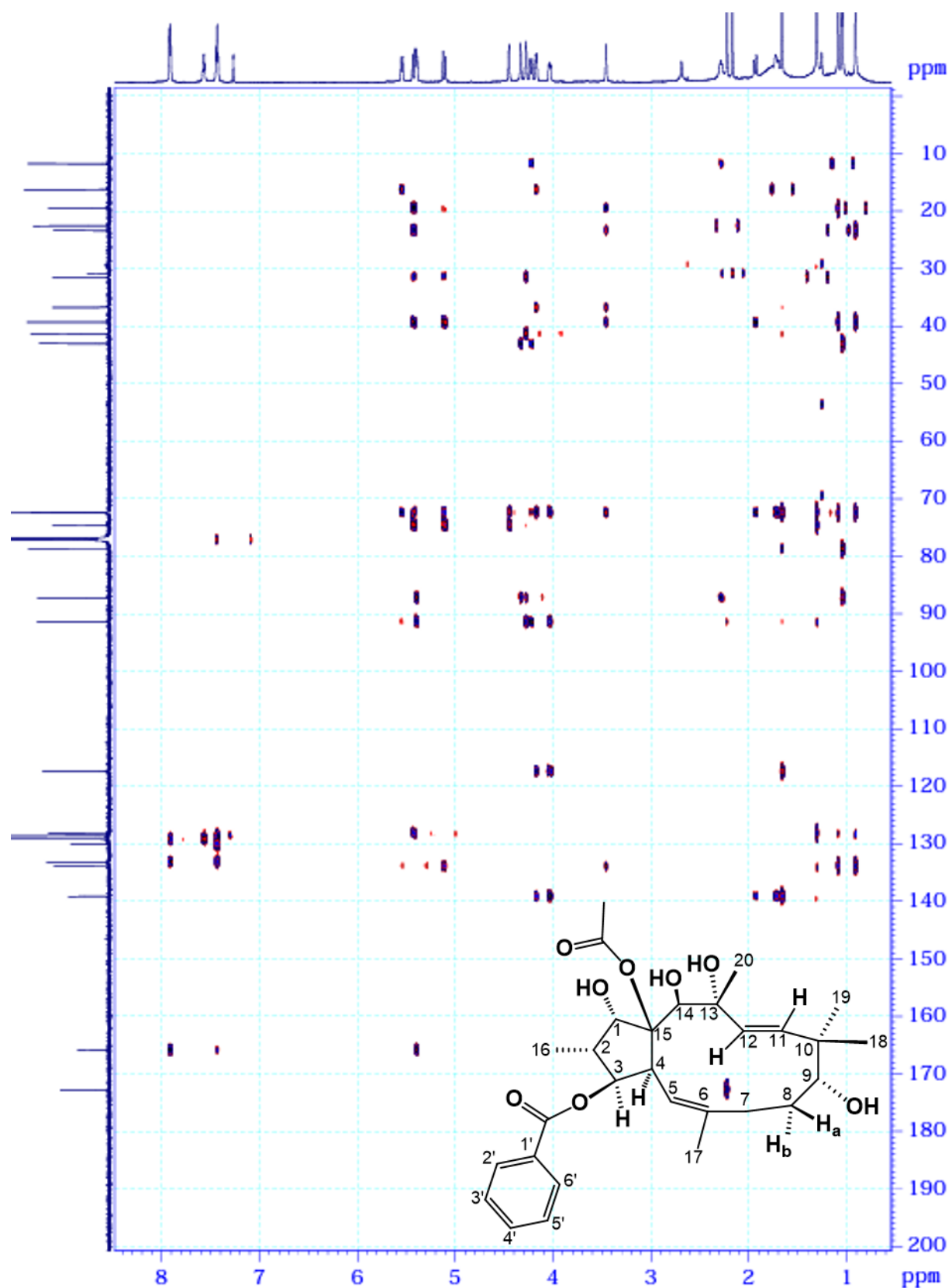


Figure S47. HMBC spectrum (sketched) of compound P5 (CDCl₃)

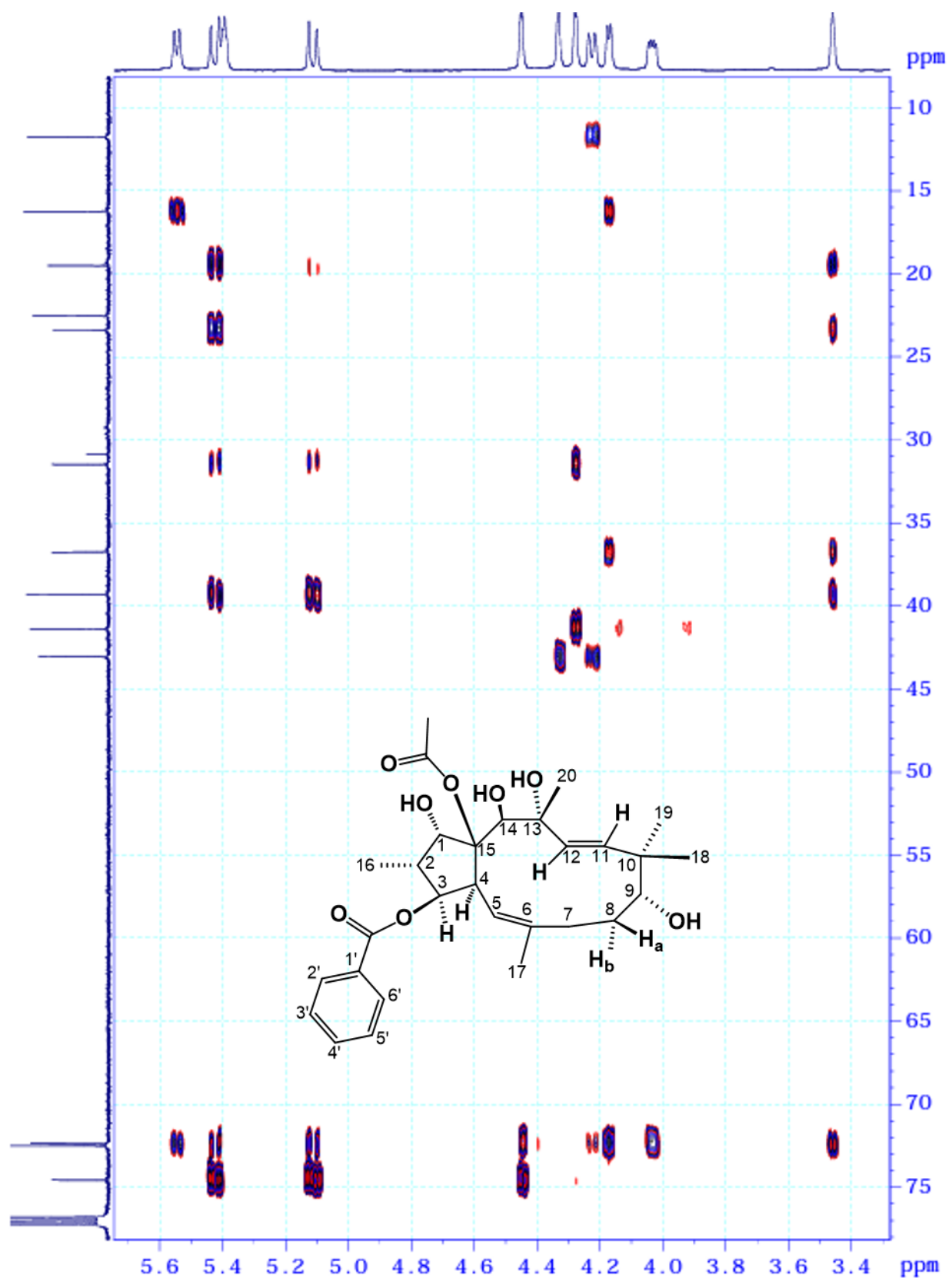


Figure S48. HMBC spectrum (sketched) of compound P5 (CDCl₃)

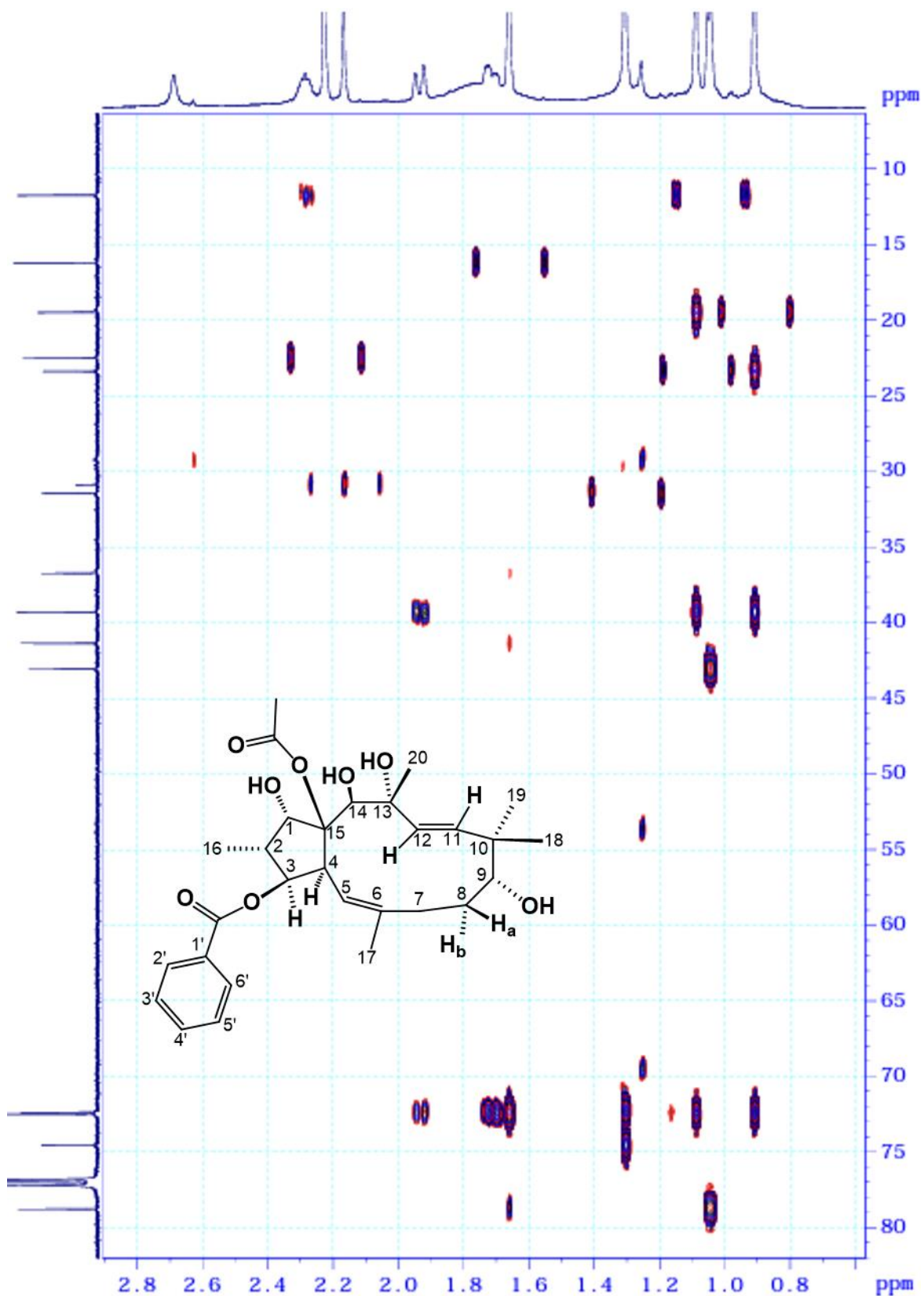


Figure S49. NOESY spectrum of compound P5 (CDCl₃)

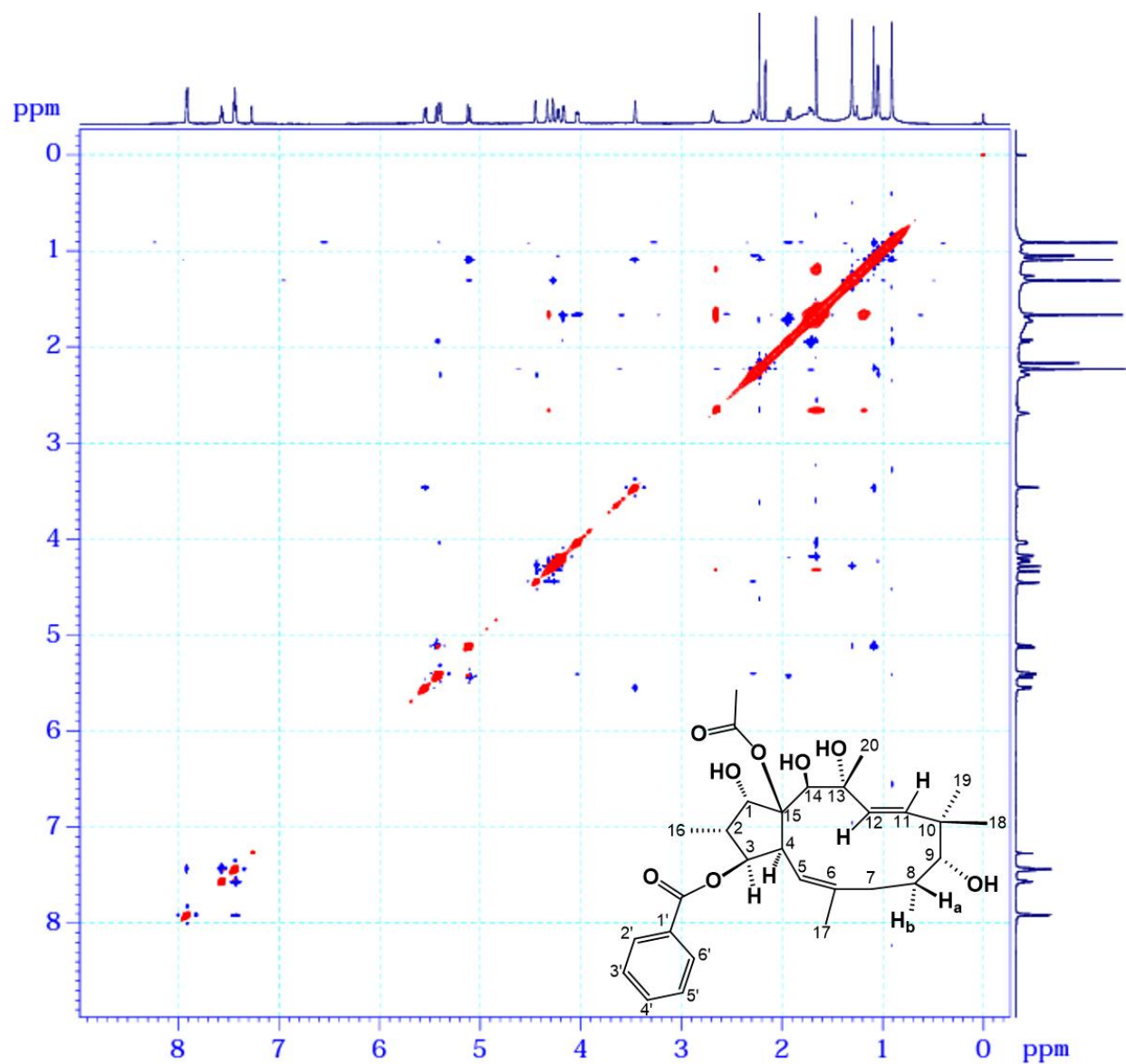


Figure S50. MS spectrum of compound P5 (CDCl_3)



Sample name: P5117
Operator: Hằng VHH
Method: +IDA TOF MS/MS
Date: 2022.10.13

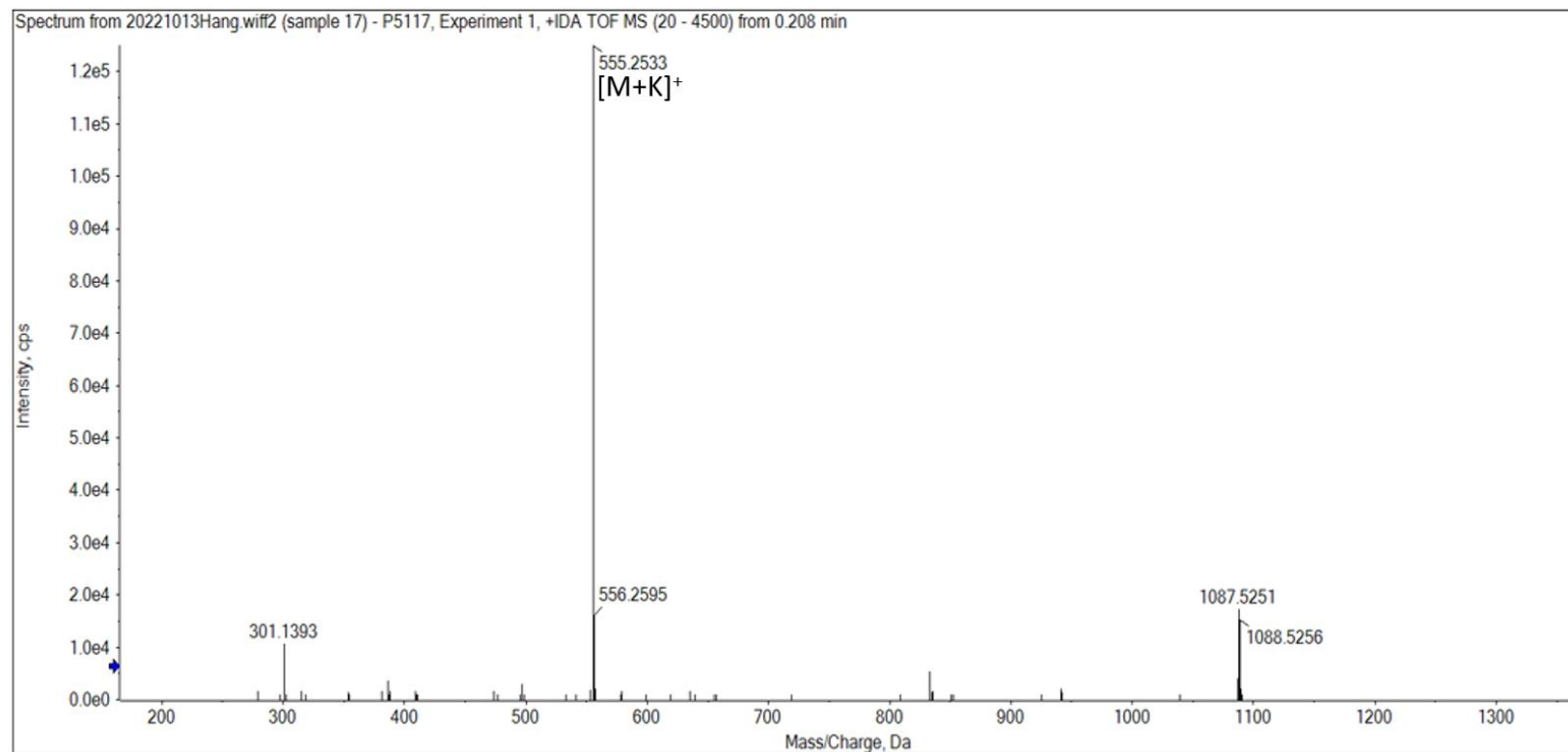


Figure S51. Structural novelty check for compound P5

Launch Meeting - Zoom x YouTube - YouTube x Facebook x Drawn Structure Substance Search x

scifinder-n.cas.org/search/substance/6373af65192c317d2fd1de4771

CAS Scifinder® Substances Enter a query...

Substances search for drawn structure

References Reactions Suppliers Save and Alert

Structure Match: As Drawn (0), Substructure (0), **Similarity (160K)**

Chemscap Analysis: Visually explore structure similarity with a powerful new tool. Learn more about Chemscap. **Create Chemscap Analysis**

Filter Behavior: Filter by Exclude

Filtering: Similarity: 3 Selected x Number of Components: 1 x Clear All Filters

181 Results Sort: Relevance View: Partial

1	2	3
2287256-51-1	1946844-10-5	1016572-85-2
Absolute stereochemistry shown E/Z labels describe double bond geometry	Absolute stereochemistry shown, Rotation (i) E/Z labels describe double bond geometry	Absolute stereochemistry shown, Rotation (i) E/Z labels describe double bond geometry
$C_{29}H_{40}O_8$ 3aH-Cyclopentacyclododecene-1,3a,4,9, 10,11-hexol, 1,2,3,4,5,8,9,10,11,13a- decaly...	$C_{27}H_{38}O_8$ 3aH-Cyclopentacyclododecene-1,3,3a,4, 5,9,11-heptol, 1,2,3,4,5,8,9,10,11,13a- deca...	$C_{29}H_{40}O_7$ 3aH-Cyclopentacyclododecene-1,3a,4,9, 11-pentol, 1,2,3,4,5,8,9,10,11,13a- decahydr...

November 15, 2022

Substances
10:25 PM

As Drawn (0)
Substructure (0)
Similarity (160K)

Rerun Search

Edit Search