

SUPPLEMENTARY INFORMATION

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

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

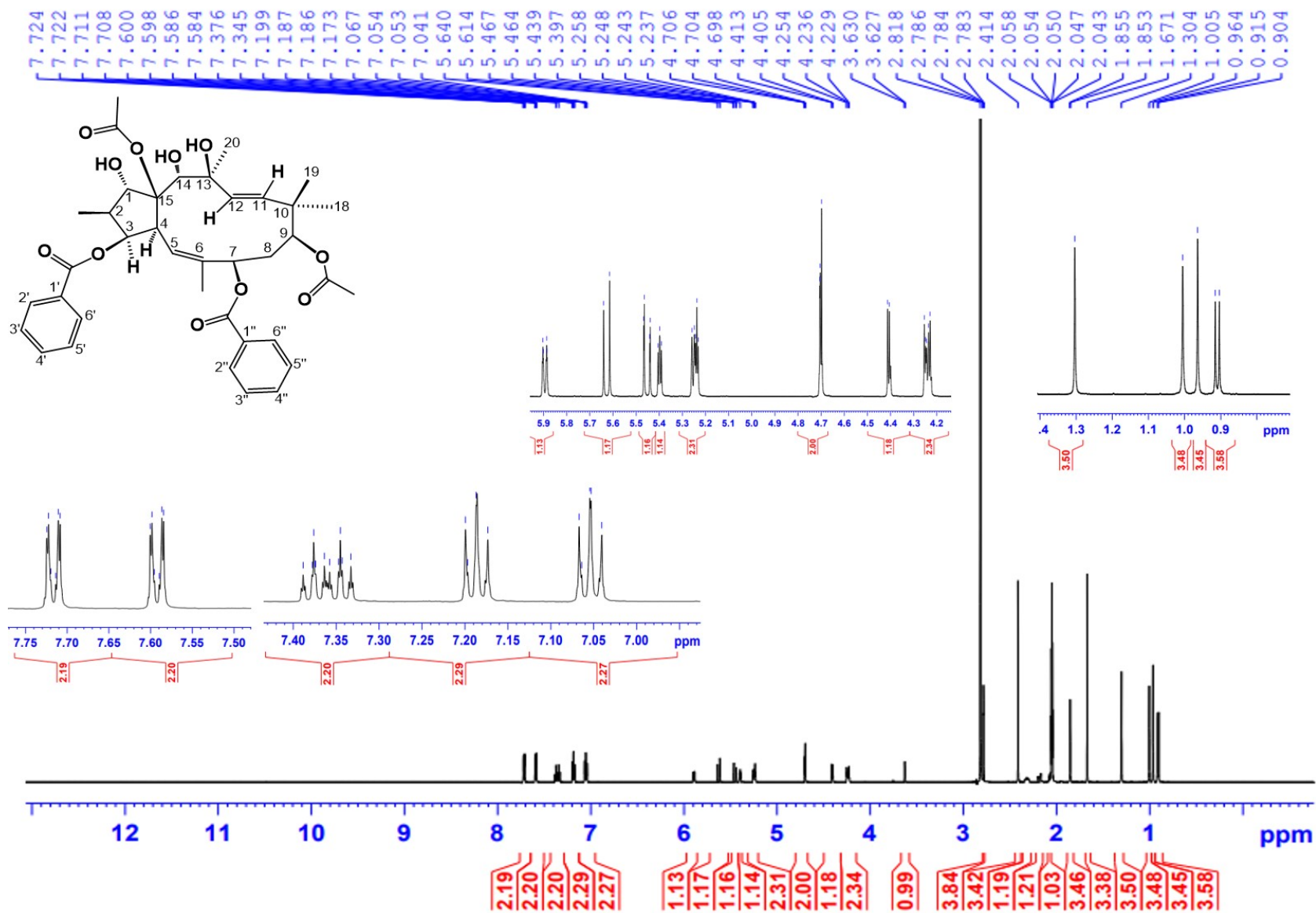


Figure S2. ^{13}C -NMR (125 MHz, Acetone- d_6) spectrum of compound P1

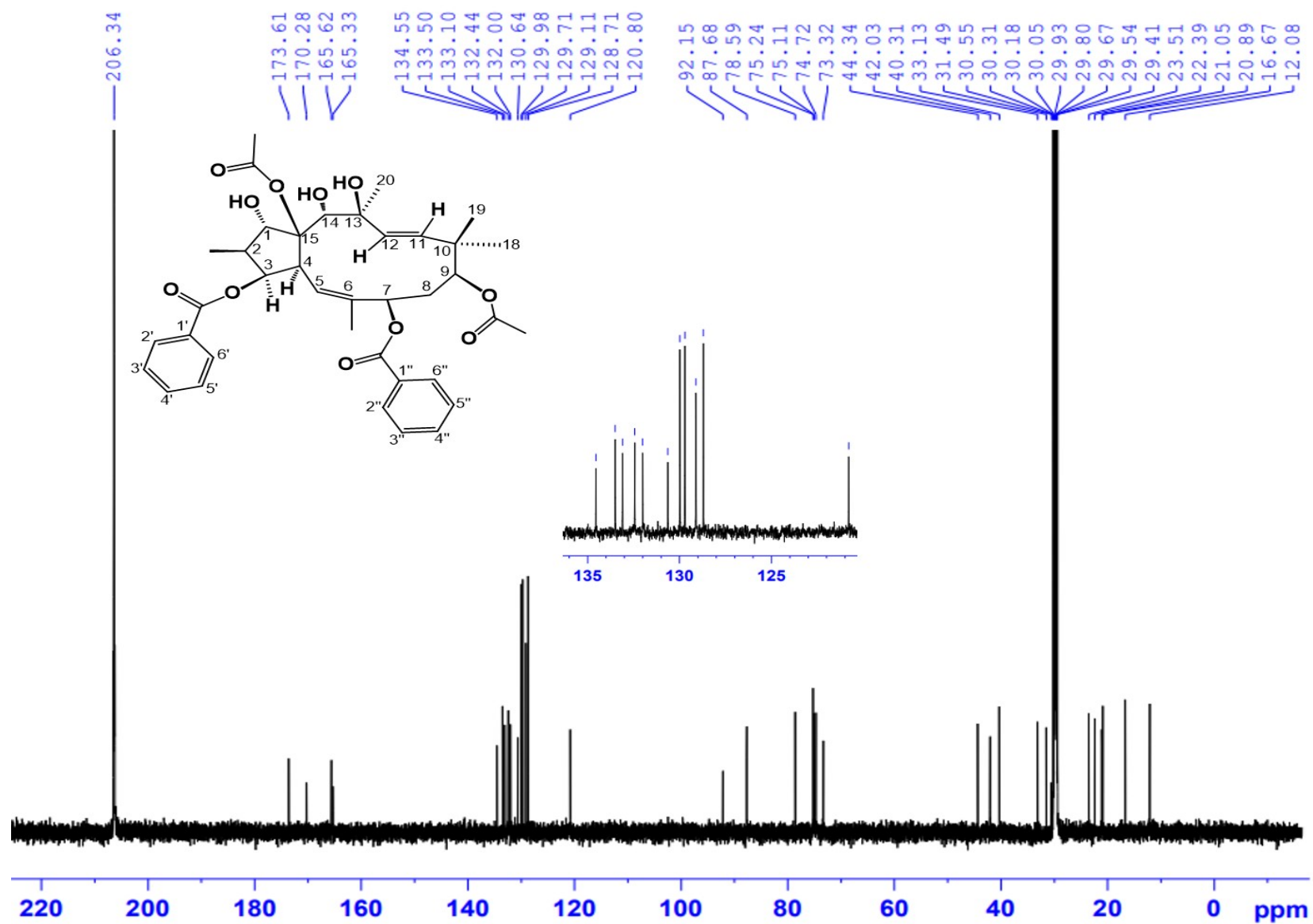


Figure S3. COSY (Acetone- d_6) spectrum of compound P1

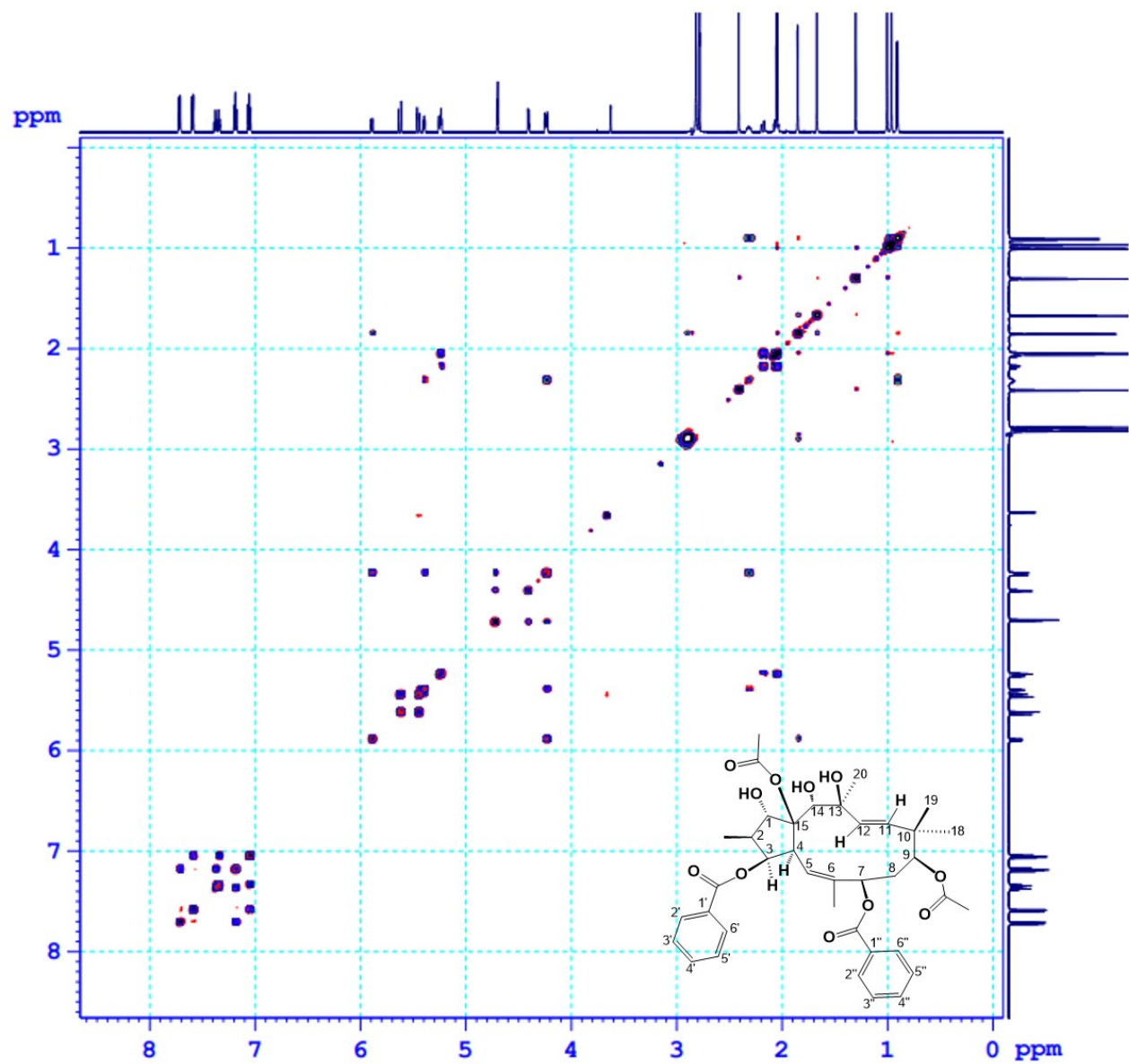


Figure S4. HSQC (Acetone- d_6) spectrum of compound P1

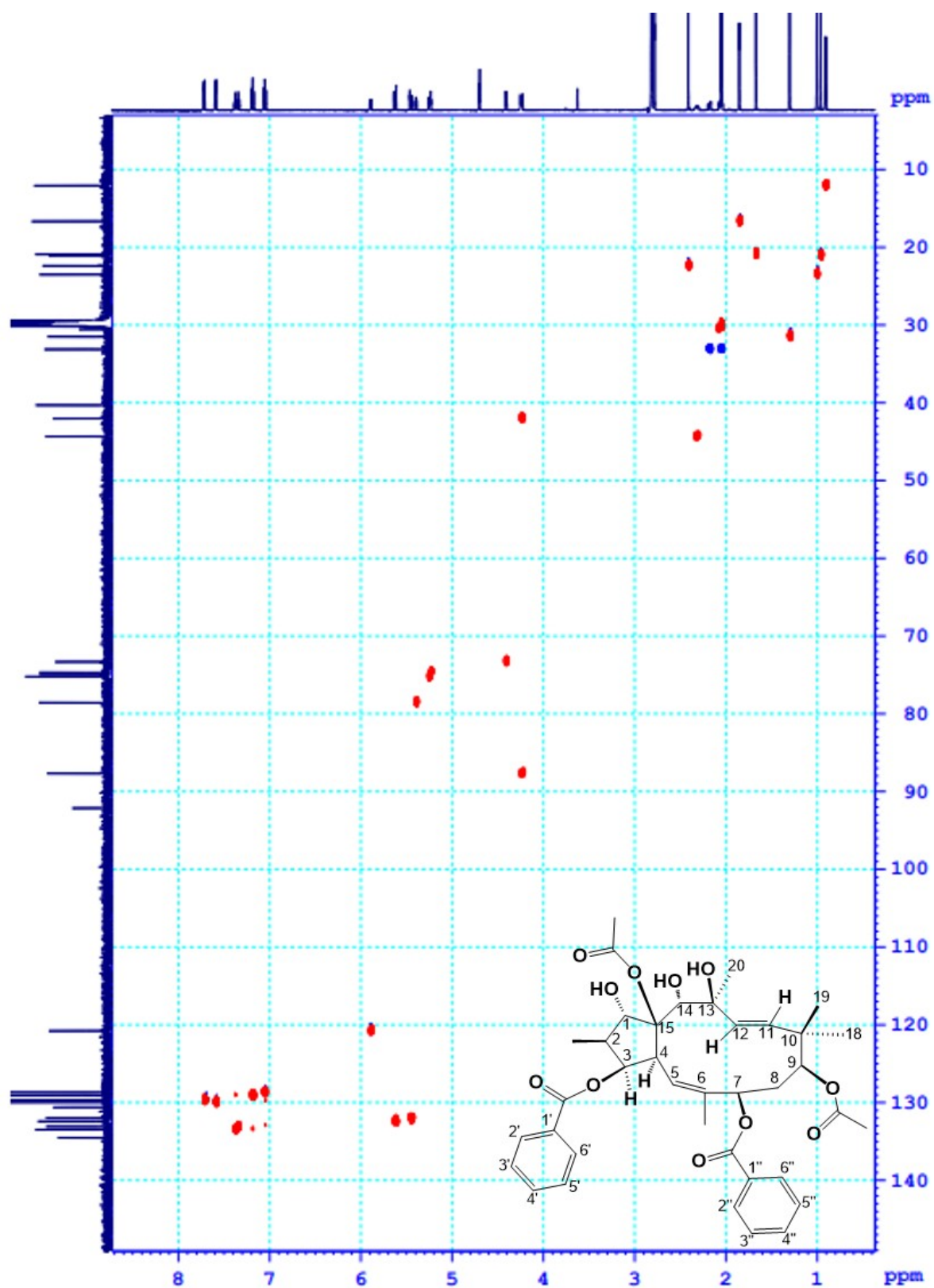


Figure S5. HMBC (Acetone- d_6) spectrum (total) of compound P1

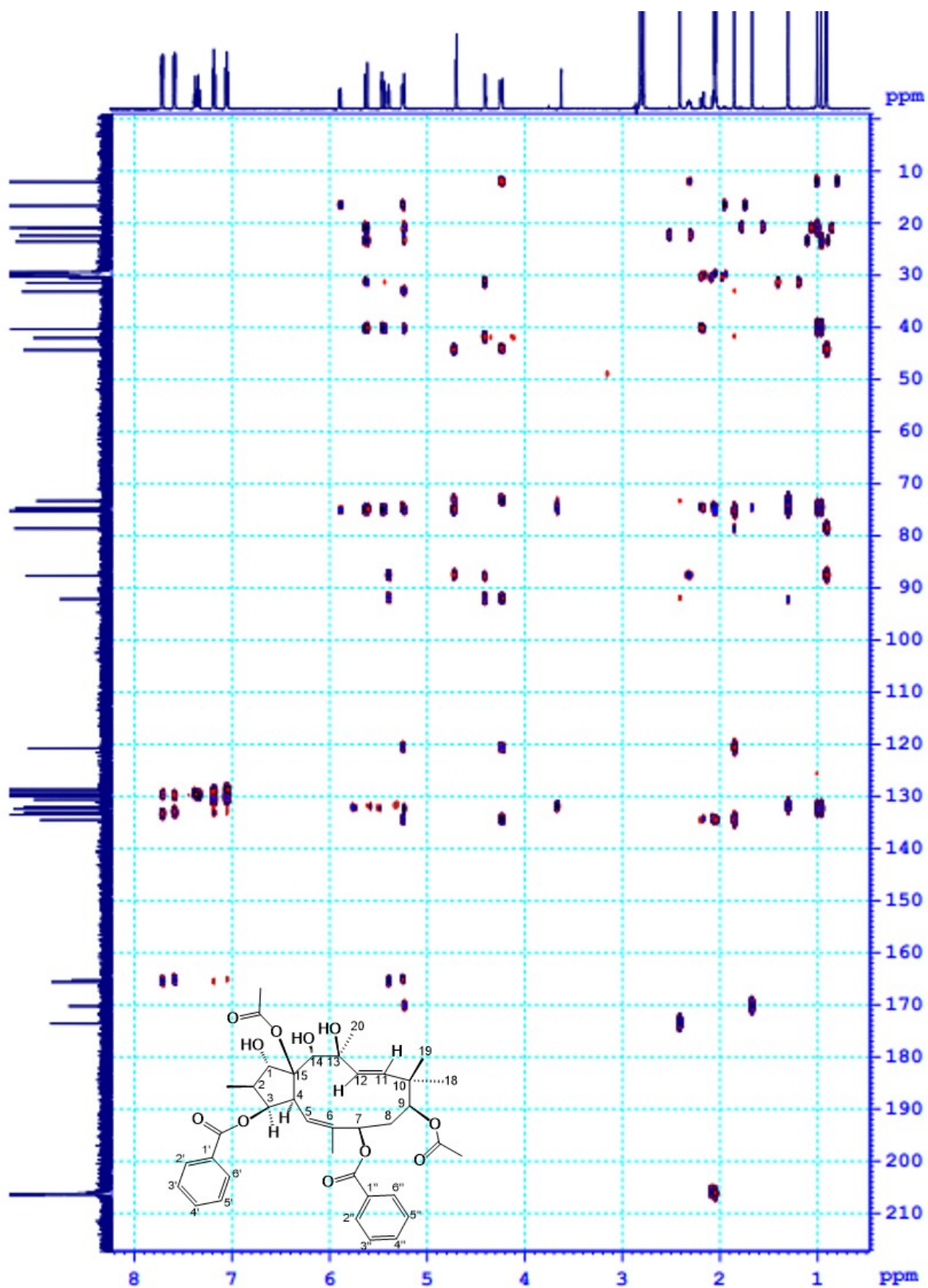


Figure S6. HMBC (Acetone- d_6) spectrum (sketched) of compound **P1**

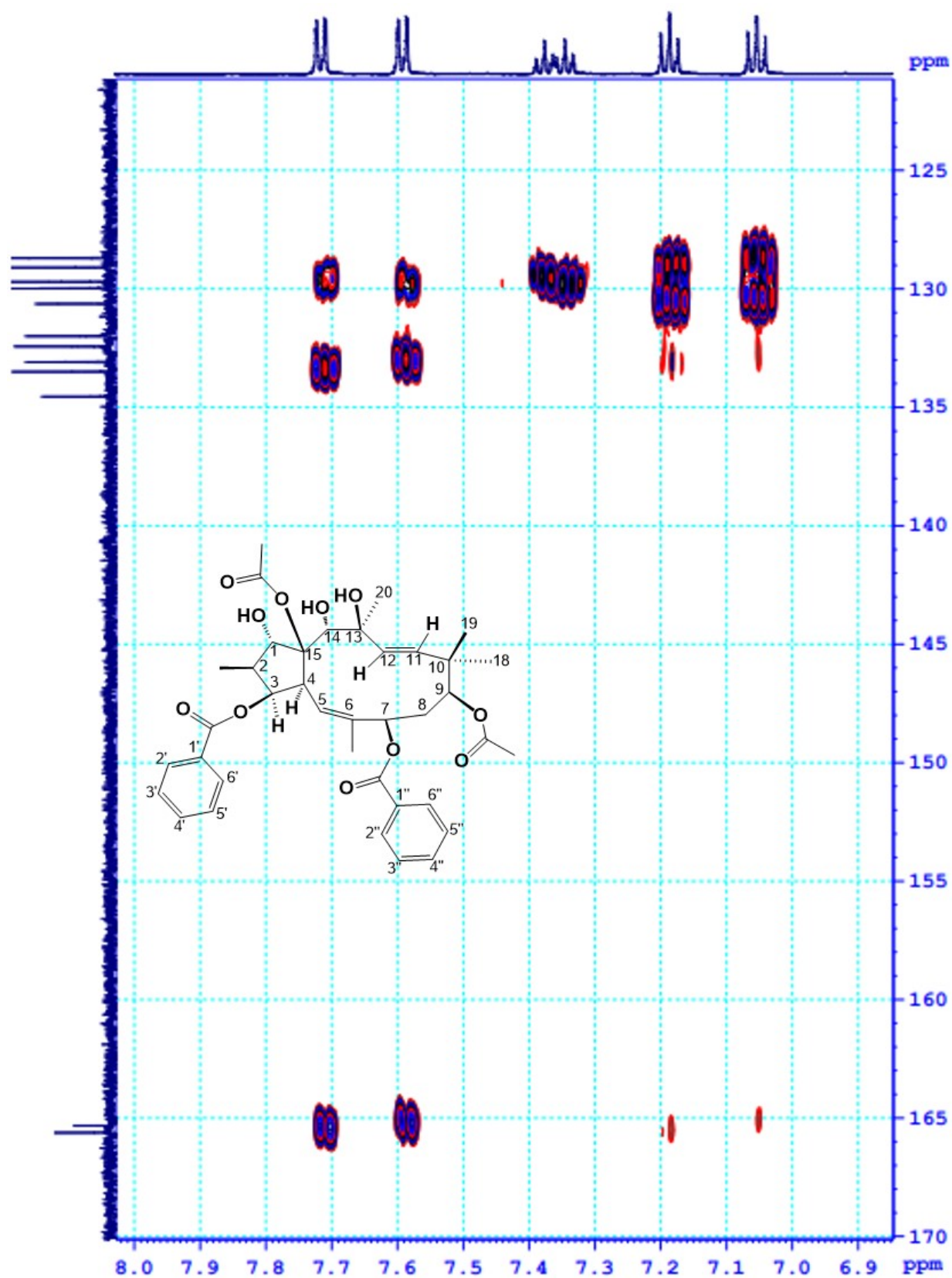


Figure S7. NOESY (Acetone- d_6) spectrum of compound P1

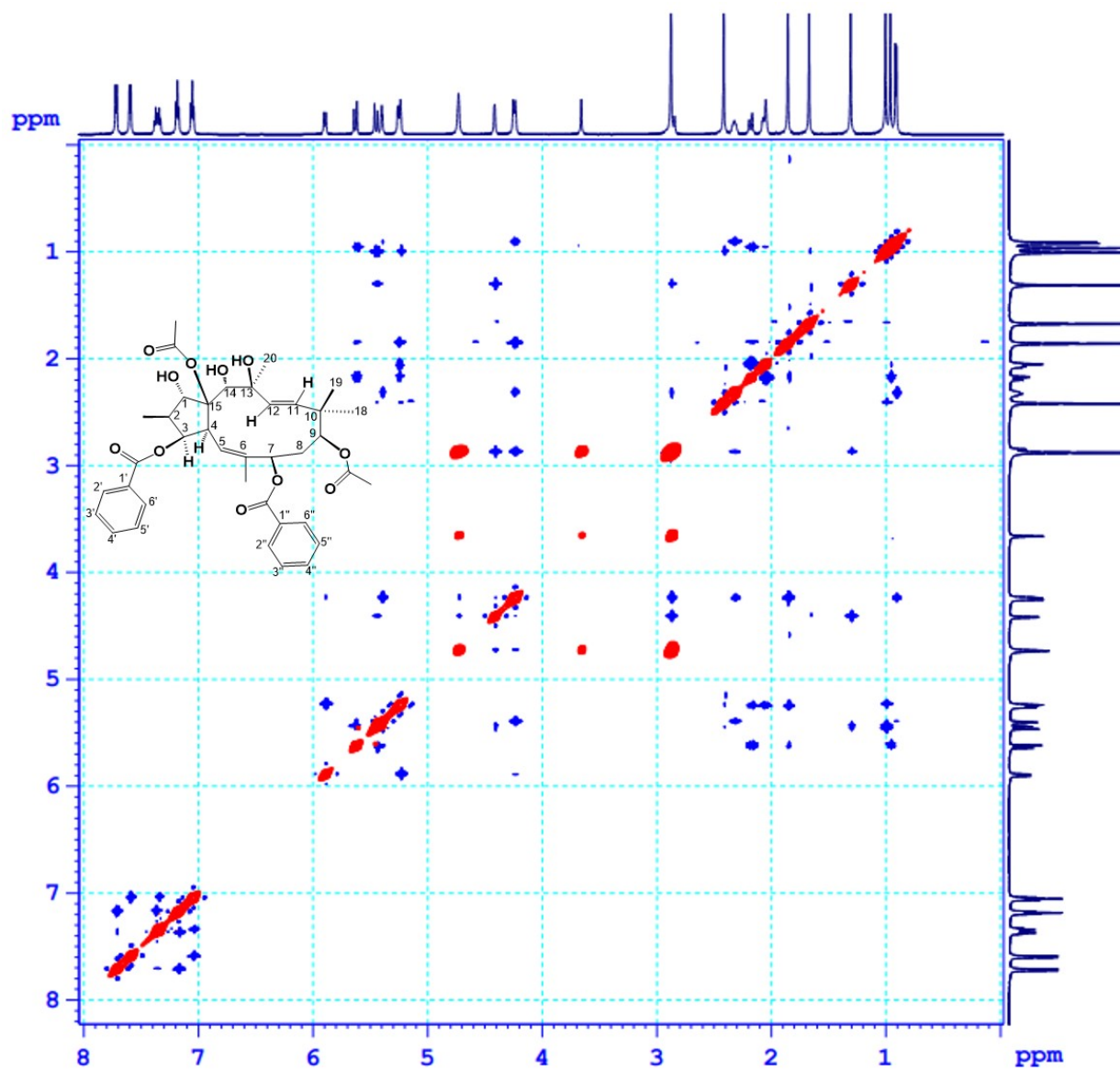


Figure S8. MS spectrum of compound P1 (Acetone- d_6)

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

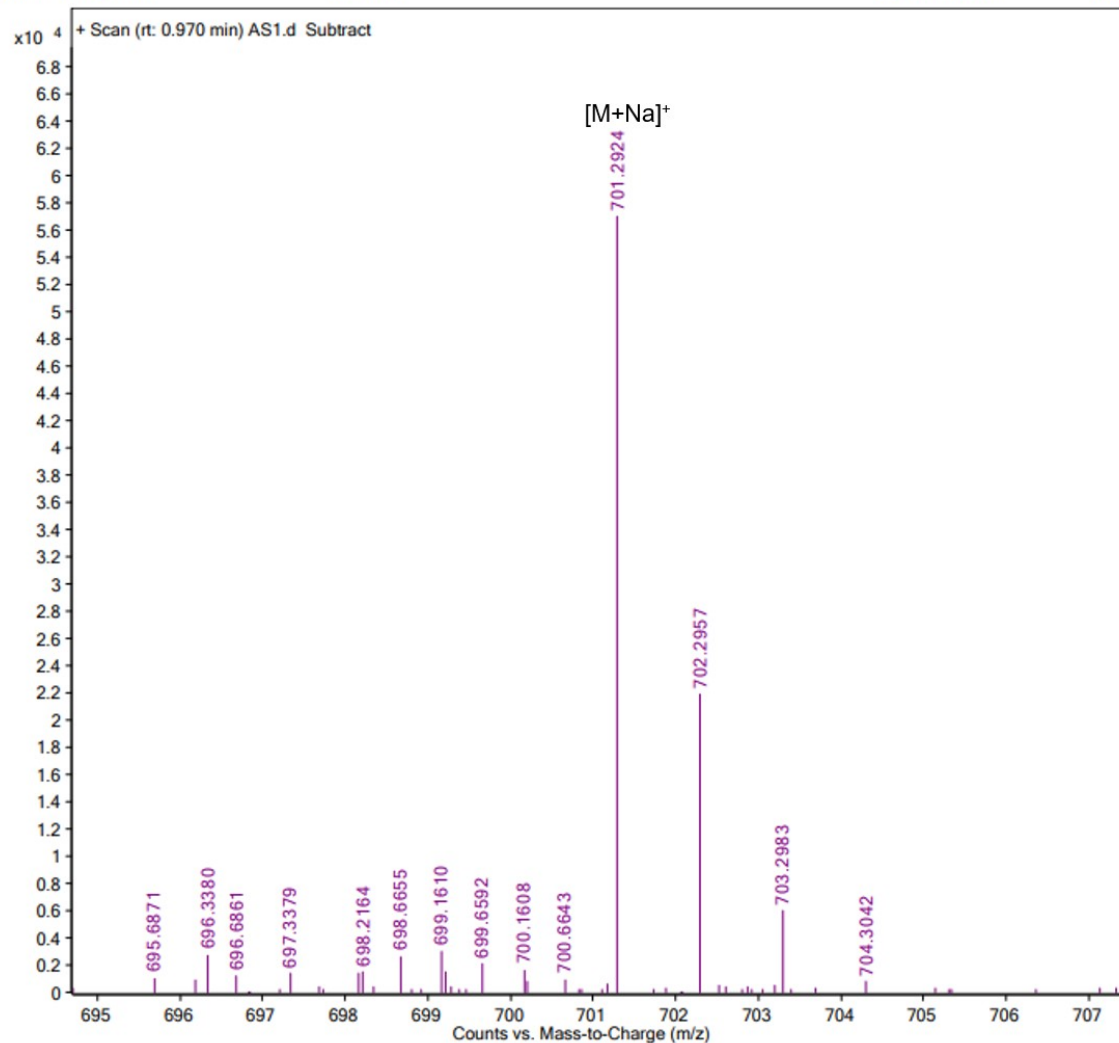


Figure S9. ¹H-NMR (600 MHz, CDCl₃) spectrum (total) of compound P2

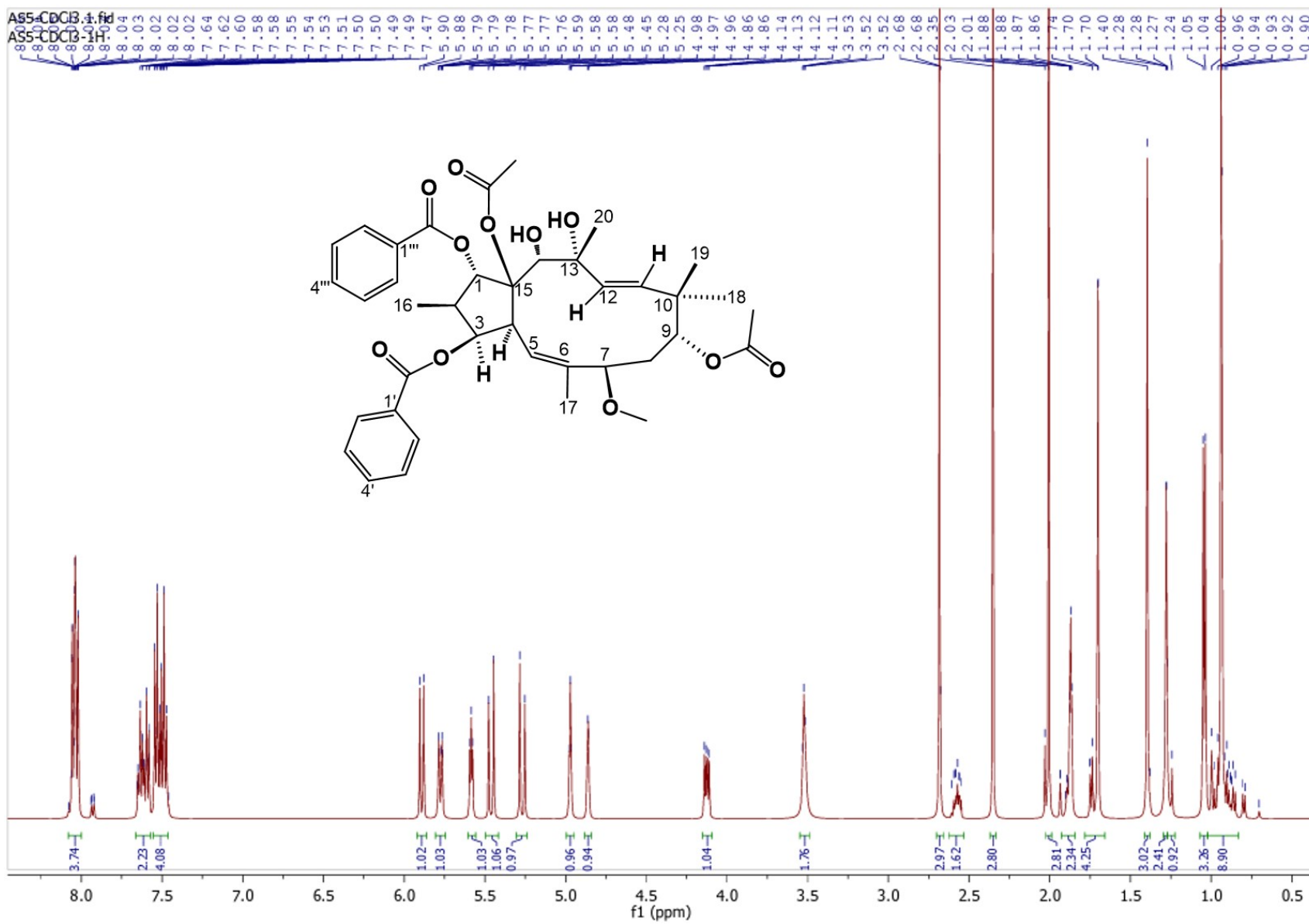


Figure S10. $^1\text{H-NMR}$ (600 MHz, CDCl_3) spectrum (sketched) of compound P2

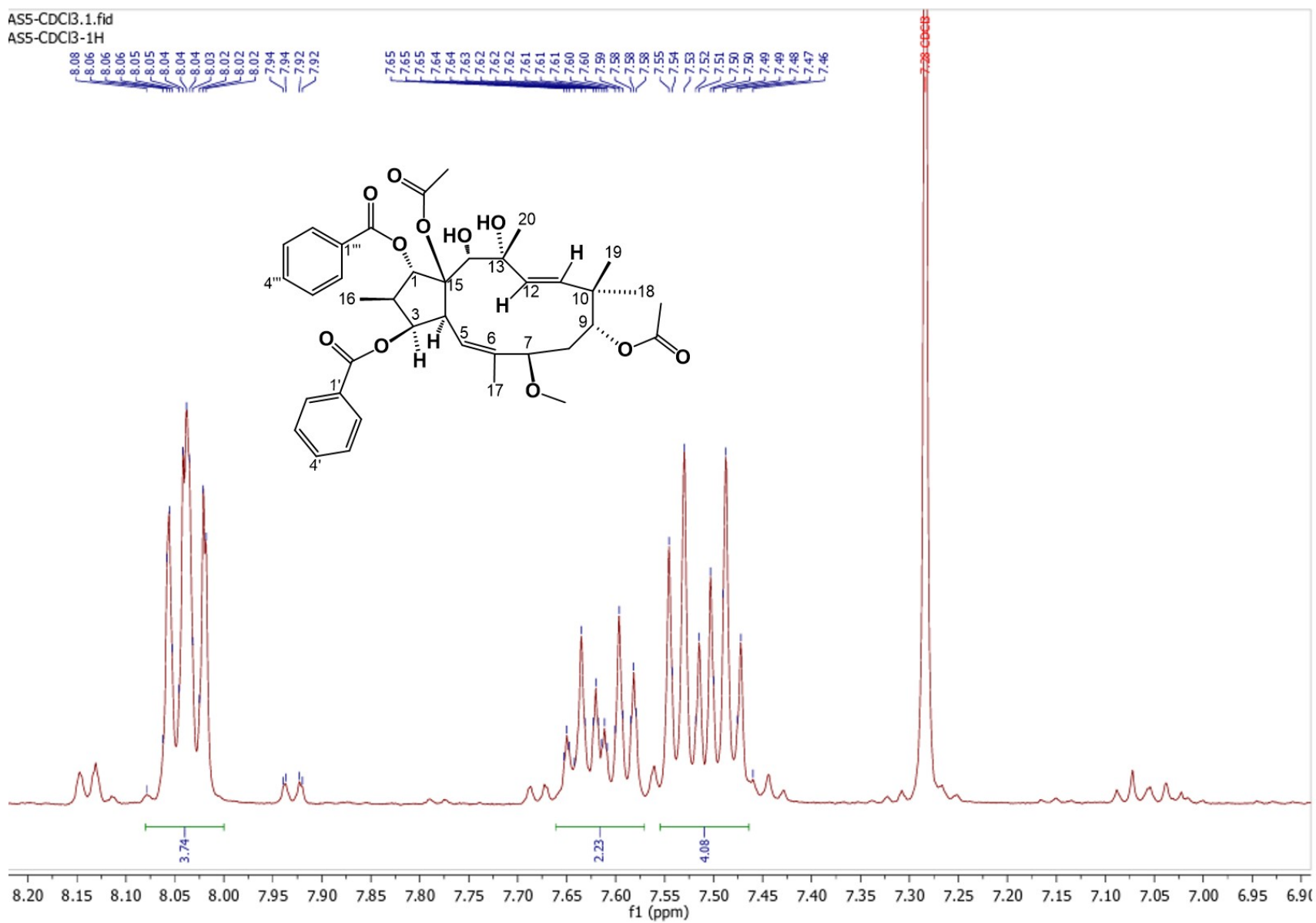


Figure S11. ¹H-NMR (600 MHz, CDCl₃) spectrum (sketched) of compound P2

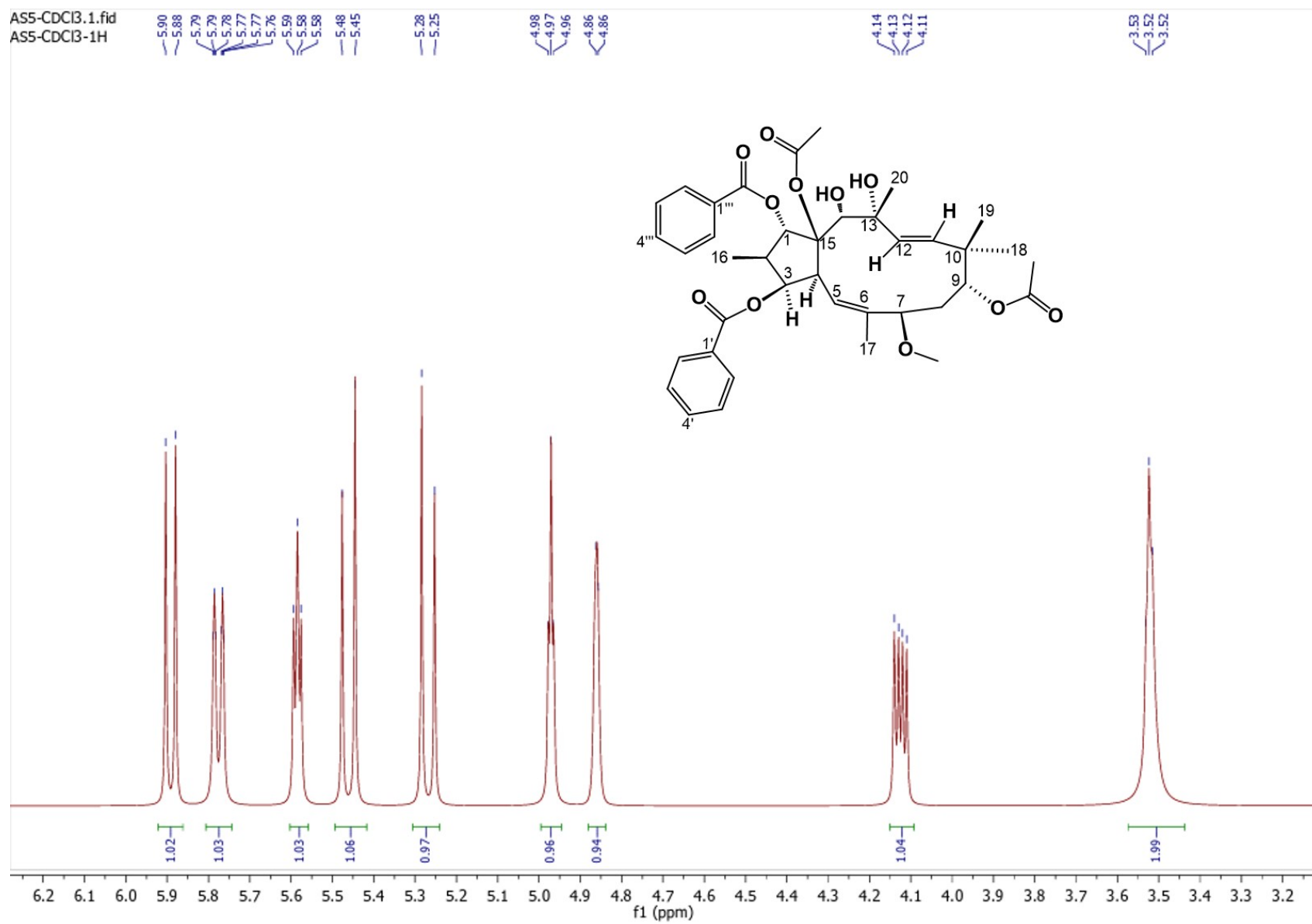


Figure S12. ¹H-NMR (600 MHz, CDCl₃) spectrum (sketched) of compound P2

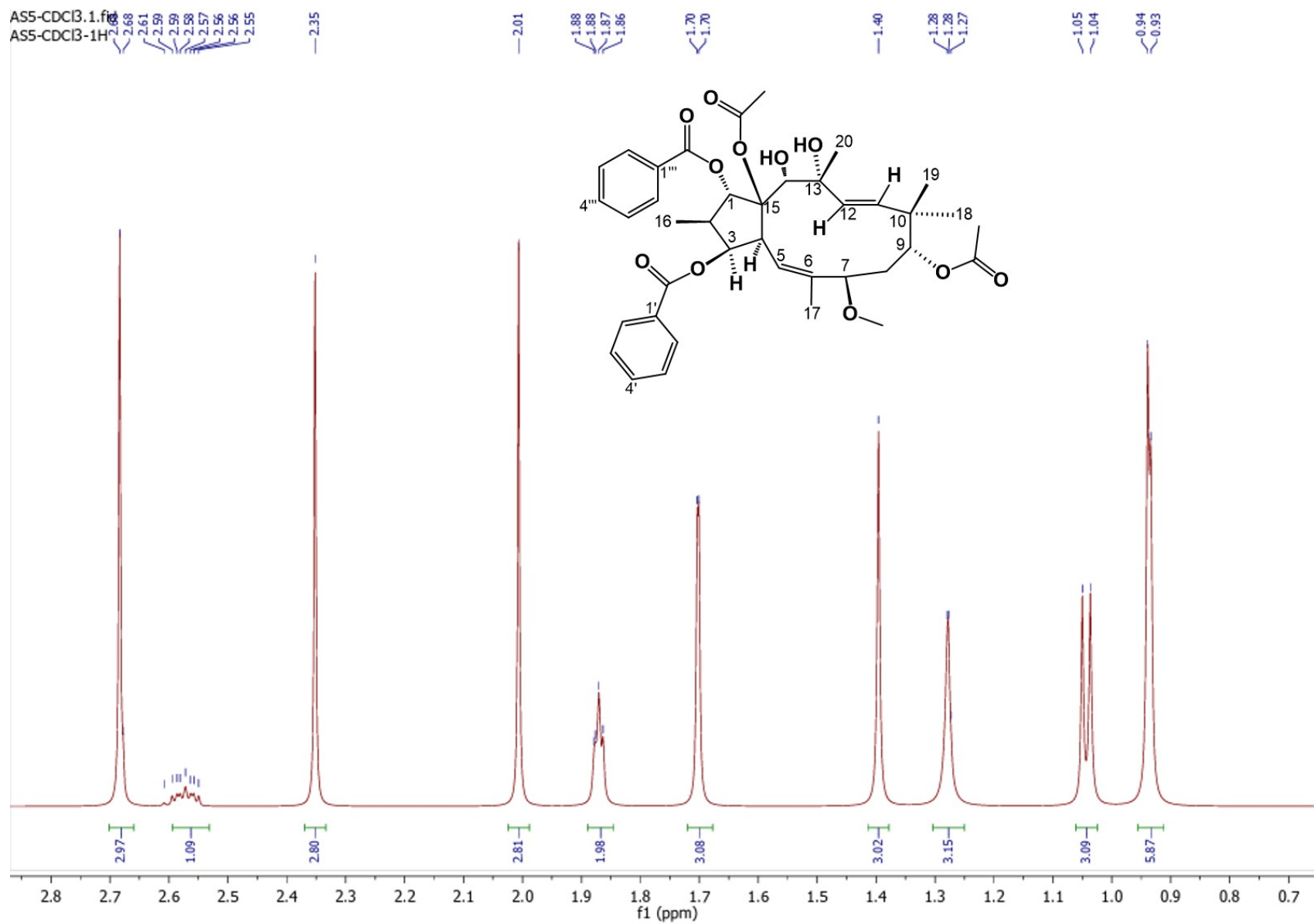


Figure S13. ^{13}C -NMR (125 MHz, CDCl_3) spectrum of compound P2

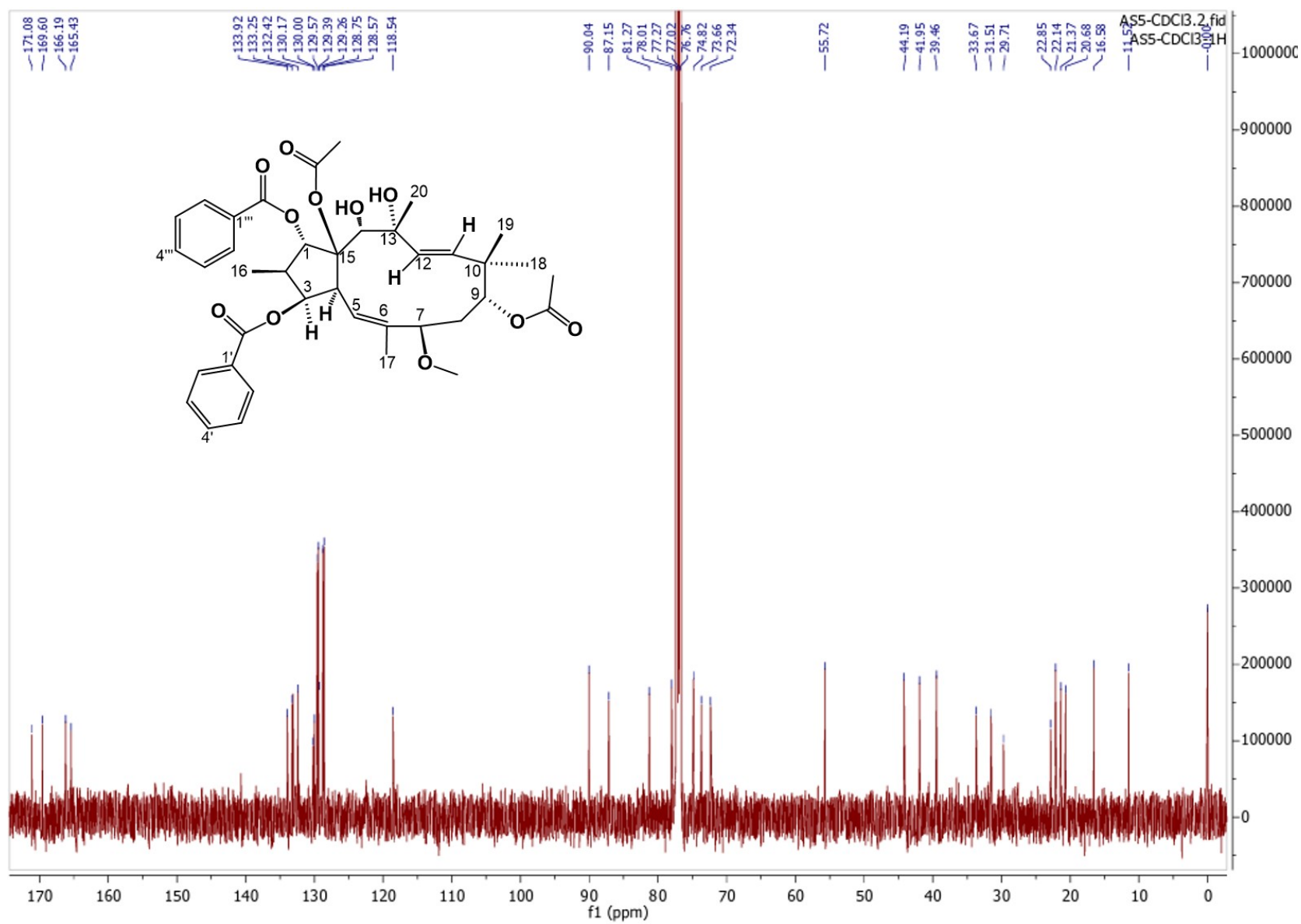


Figure S14. COSY (CDCl₃) spectrum of compound P2

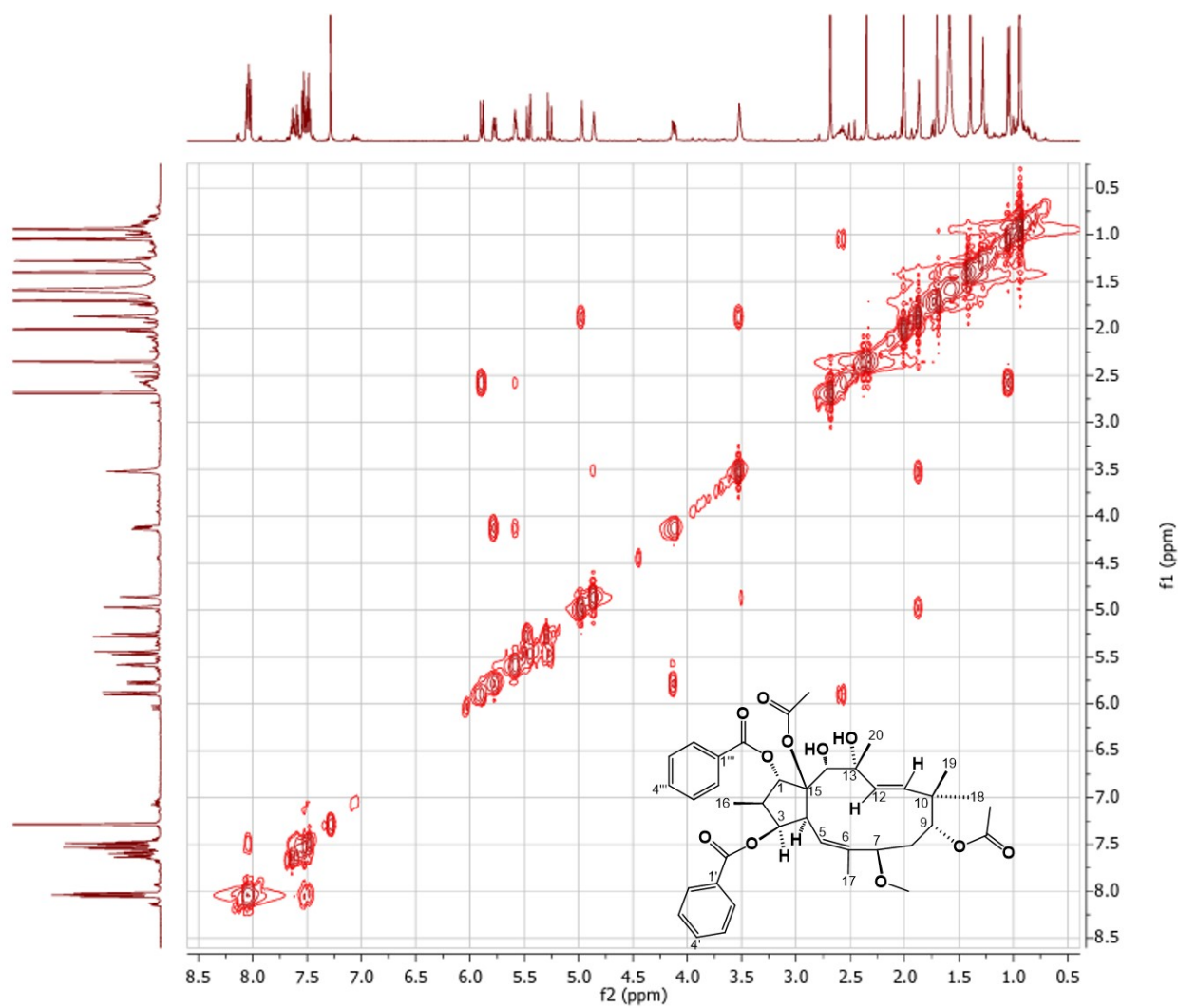


Figure S15. HSQC (CDCl₃) spectrum of compound P2

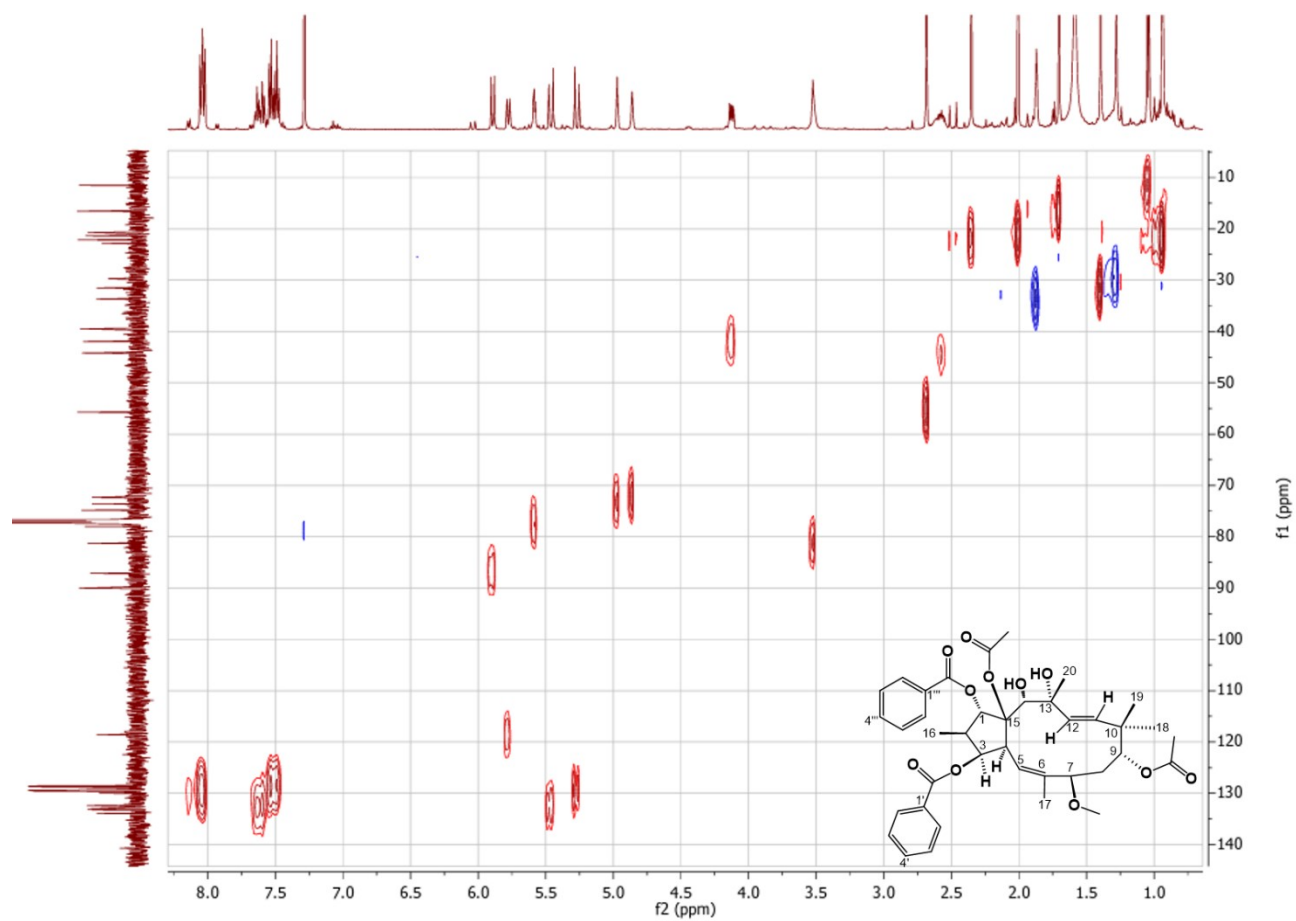


Figure S16. HMBC (CDCl₃) spectrum of compound P2

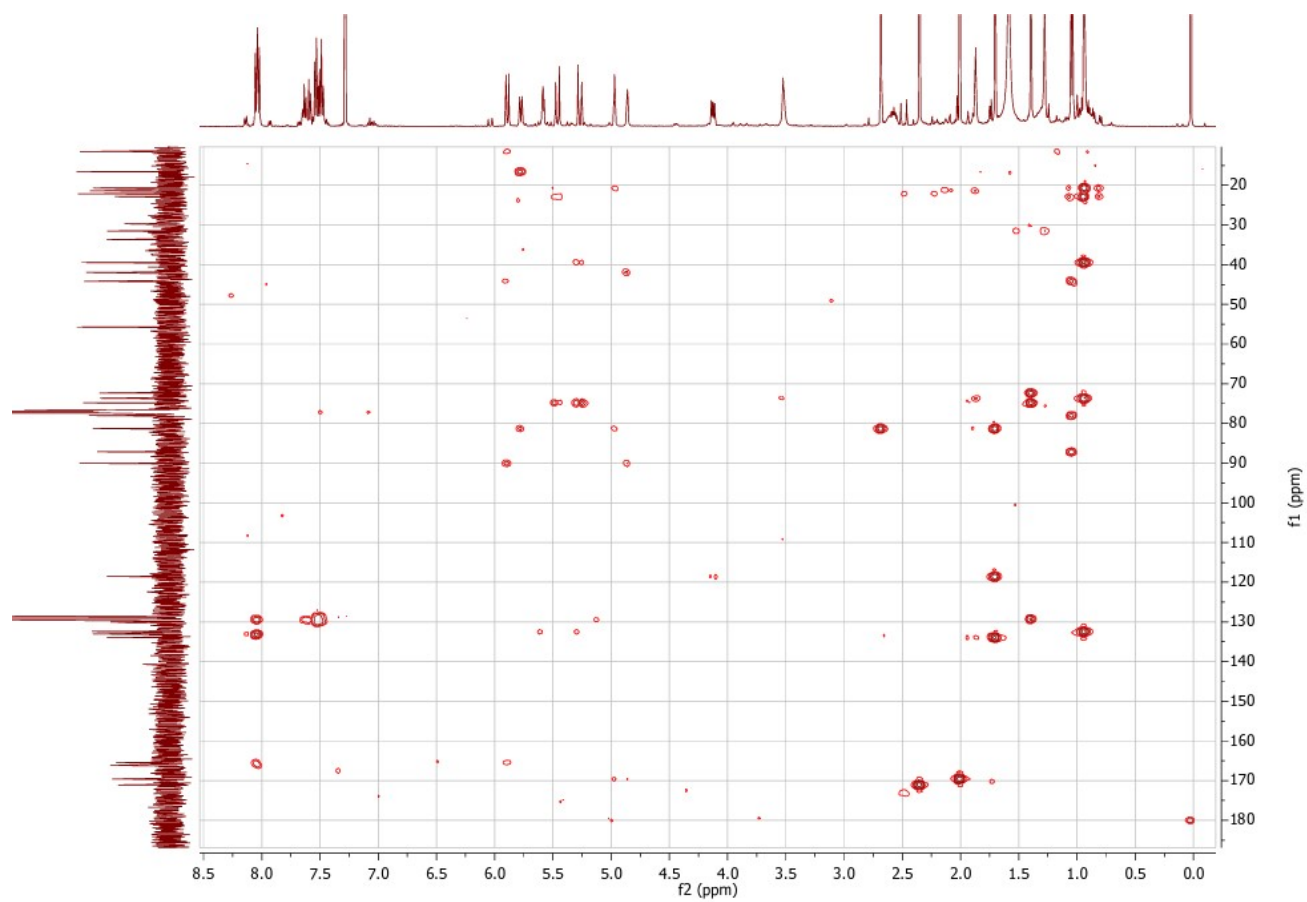


Figure S17. NOESY (CDCl₃) spectrum of compound P2

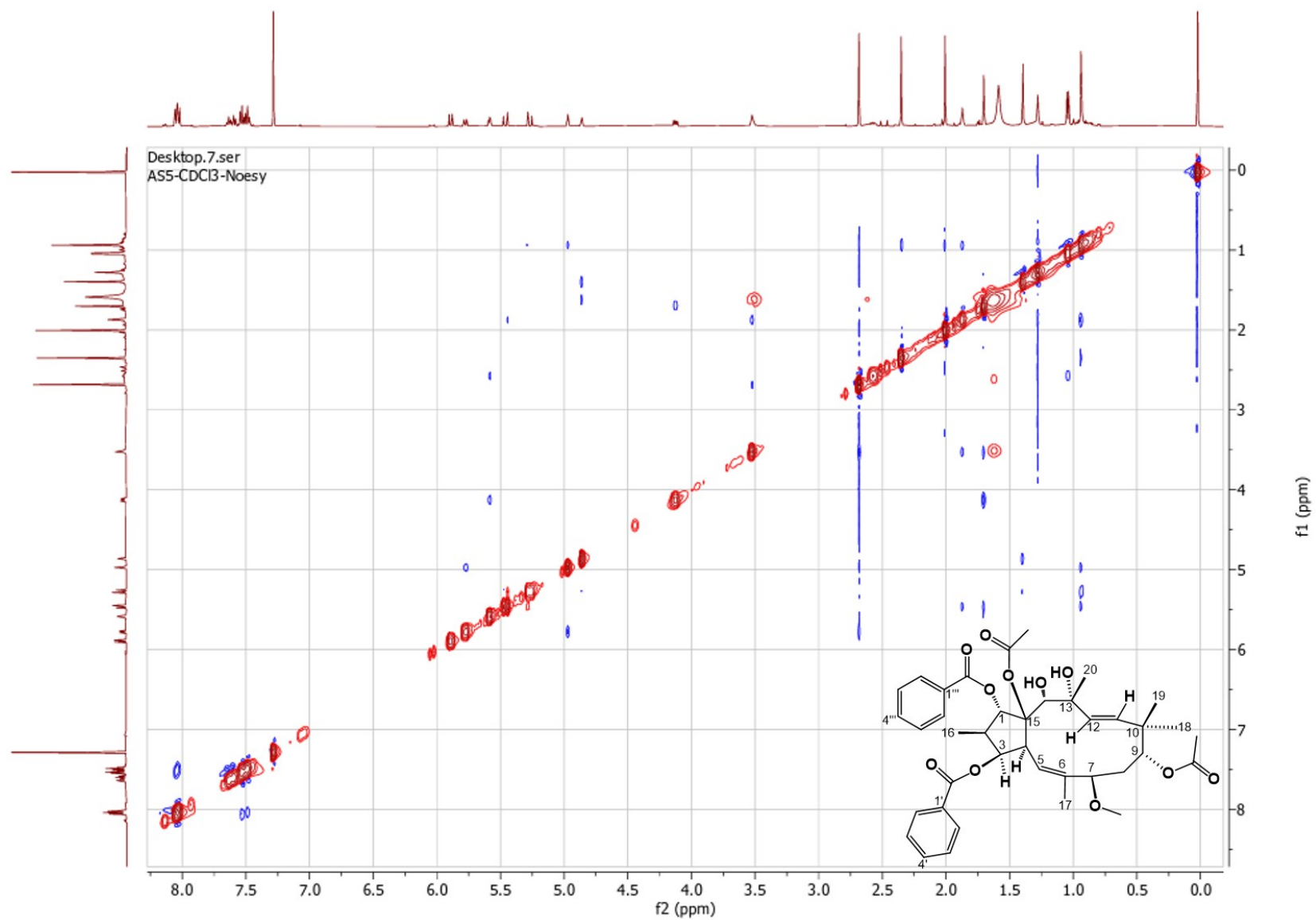
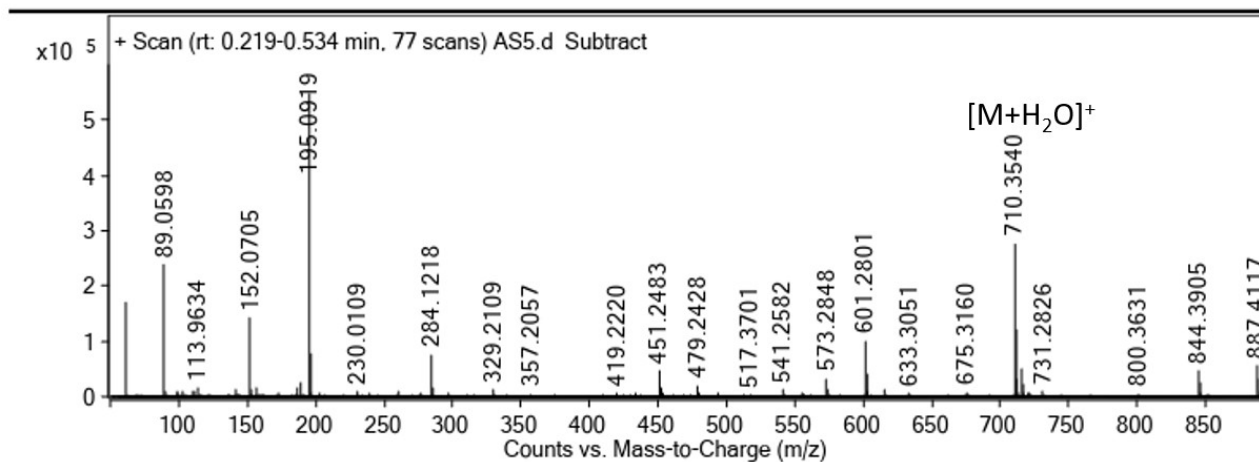


Figure S18. MS spectrum of compound P2 (CDCl₃)

Qualitative Analysis Report



Peak List

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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

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Structure Match

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- Substructure (2)**
- Similarity (155K)

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Filter Behavior

2 Results Sort: Relevance View: Partial

1

1946844-18-3

Absolute stereochemistry shown, Rotation (-)
E/Z labels describe double bond geometry

$C_{45}H_{50}O_{12}$

2 References 2 Reactions 1 Supplier

2

1946844-15-0

Absolute stereochemistry shown, Rotation (-)
E/Z labels describe double bond geometry

$C_{45}H_{49}BrO_{12}$

Benzoic acid, 4-bromo-, (1S,2R,3S,3aS,4E,6R,8R,10E,12R,13R,13aR)-8,13a-bis(acety...

2 References 2 Reactions 1 Supplier

Feedback

100% 27°C ENG 10:35 PM

Substances 10:35 PM

As Drawn (0)
Substructure (2)
Similarity (155K)

Rerun Search

Edit Search

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

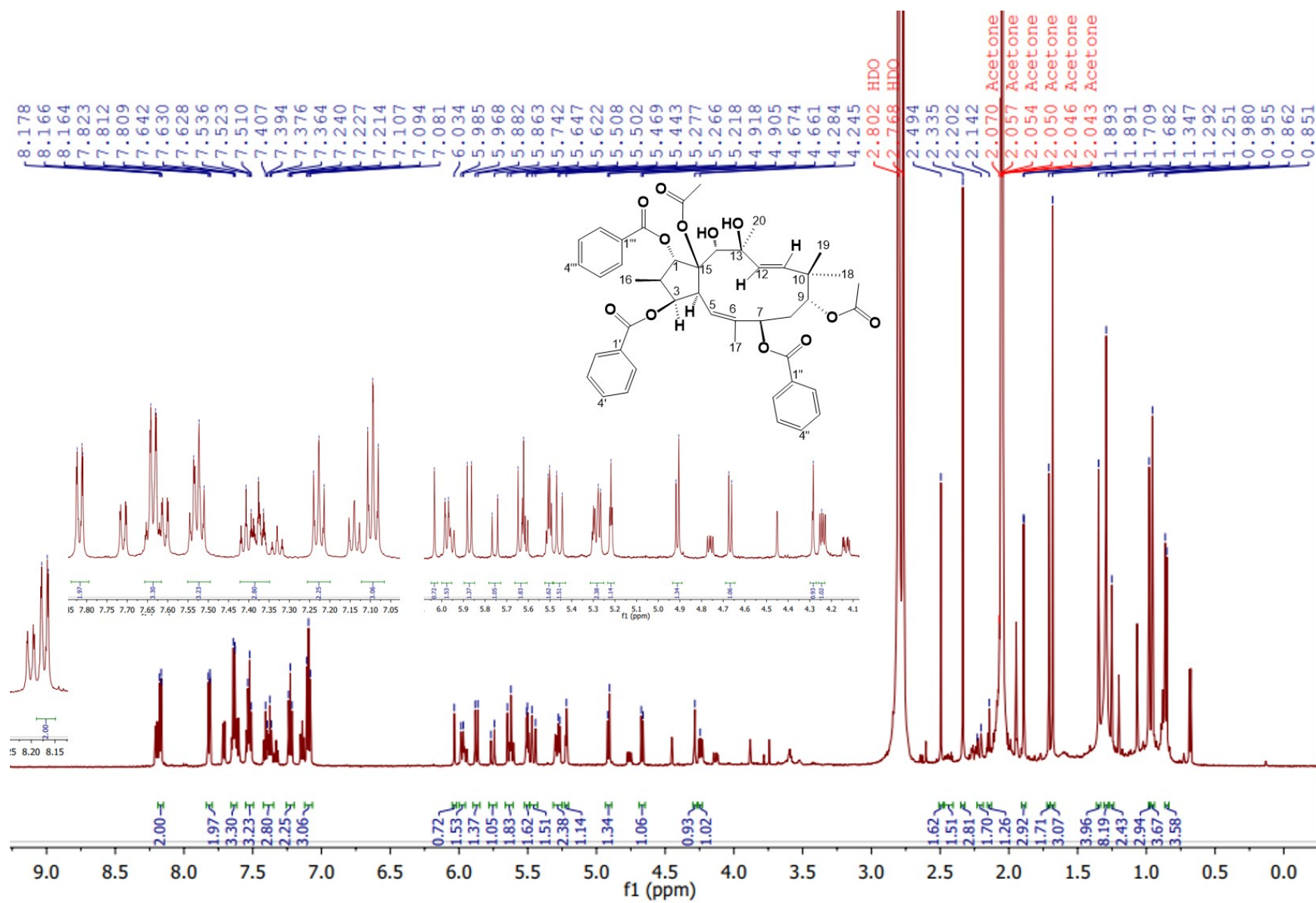


Figure S21. $^1\text{H-NMR}$ (600 MHz, Acetone- d_6) (sketched) spectrum of compound **P3**

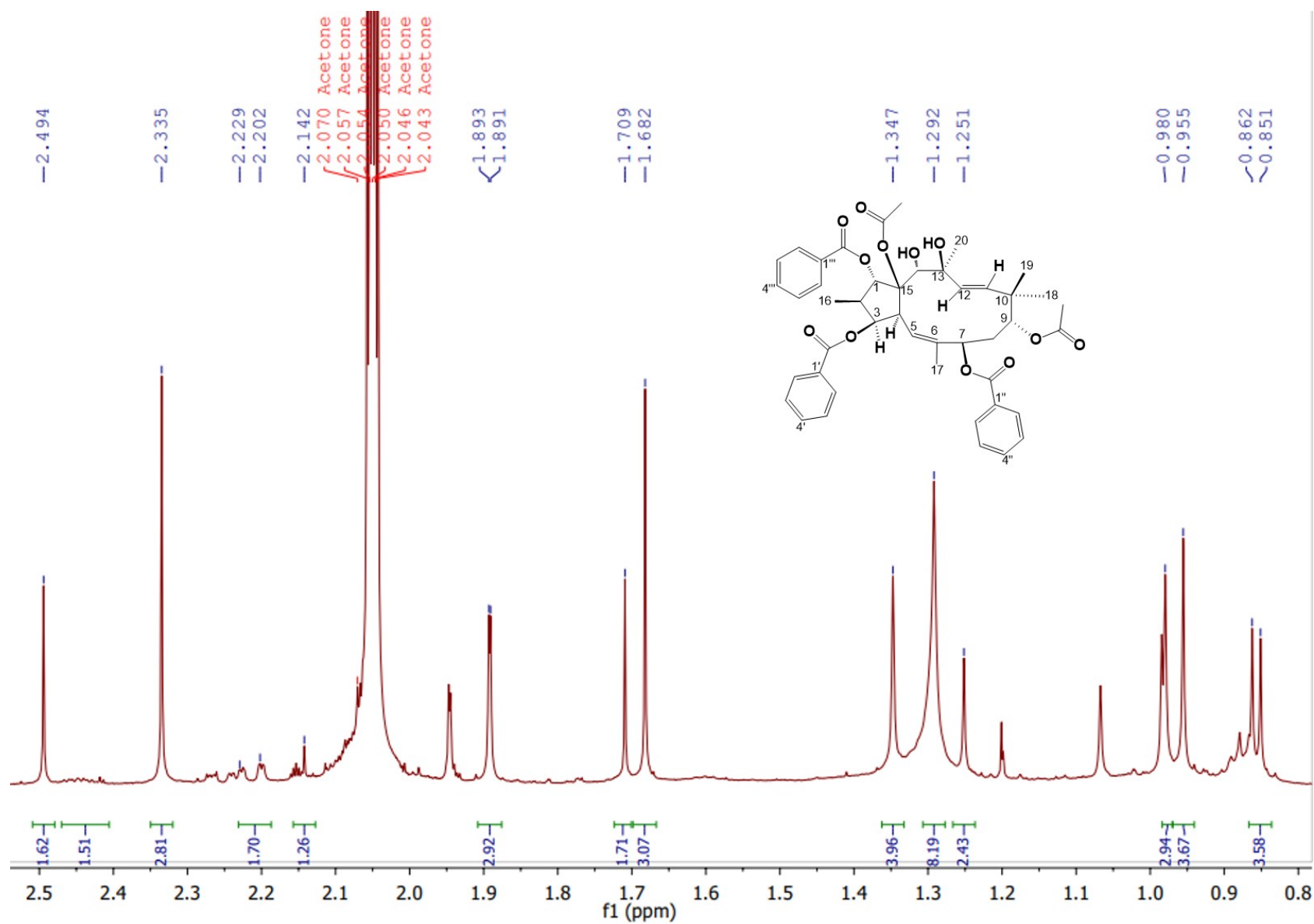


Figure S22. ^{13}C -NMR (125 MHz, Acetone- d_6) spectrum of compound P3

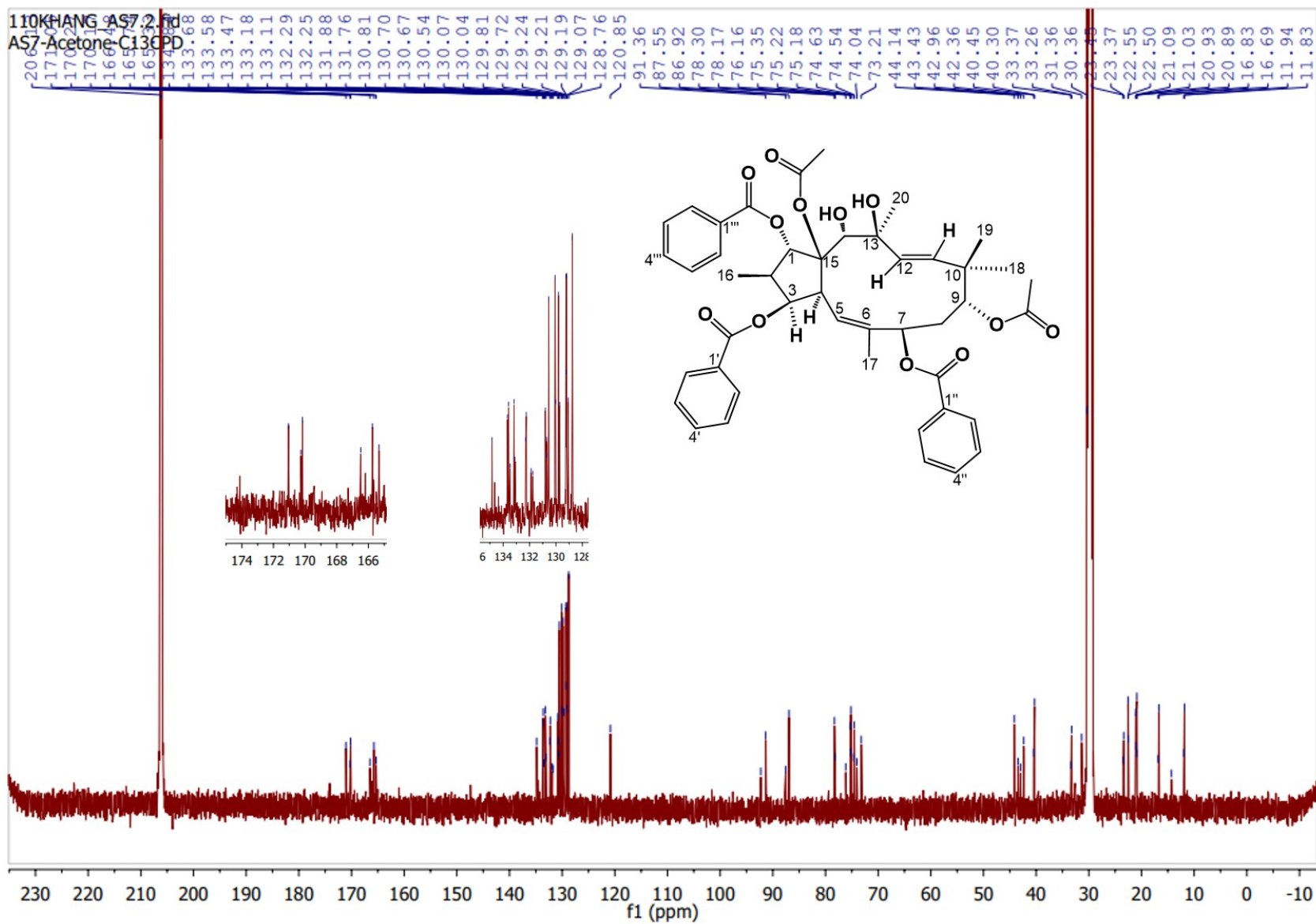


Figure S23. COSY spectrum of compound **P3** (Acetone- d_6)

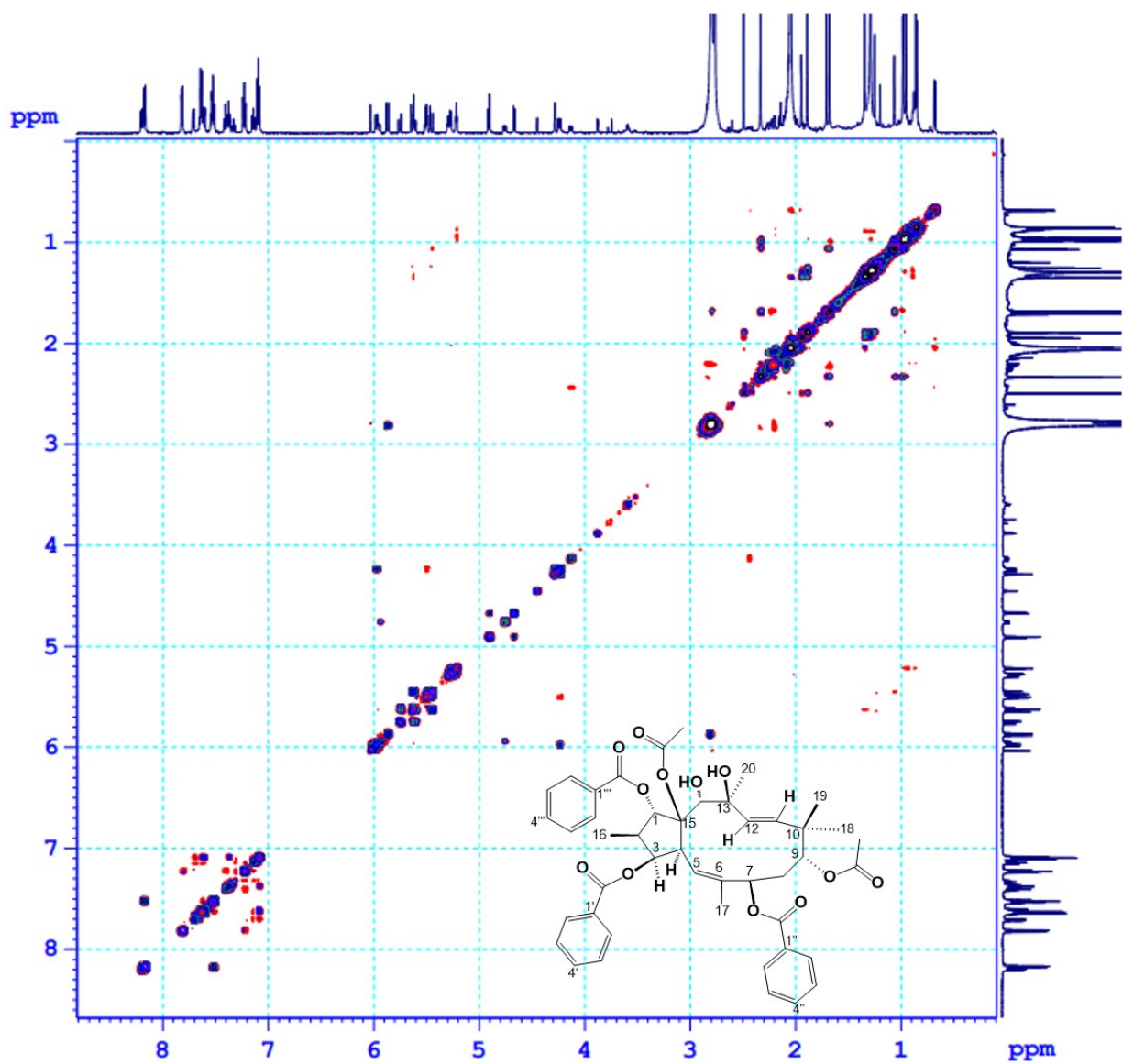


Figure S24. HSQC spectrum (total) of compound **P3** (Acetone- d_6)

AS07 HSQC

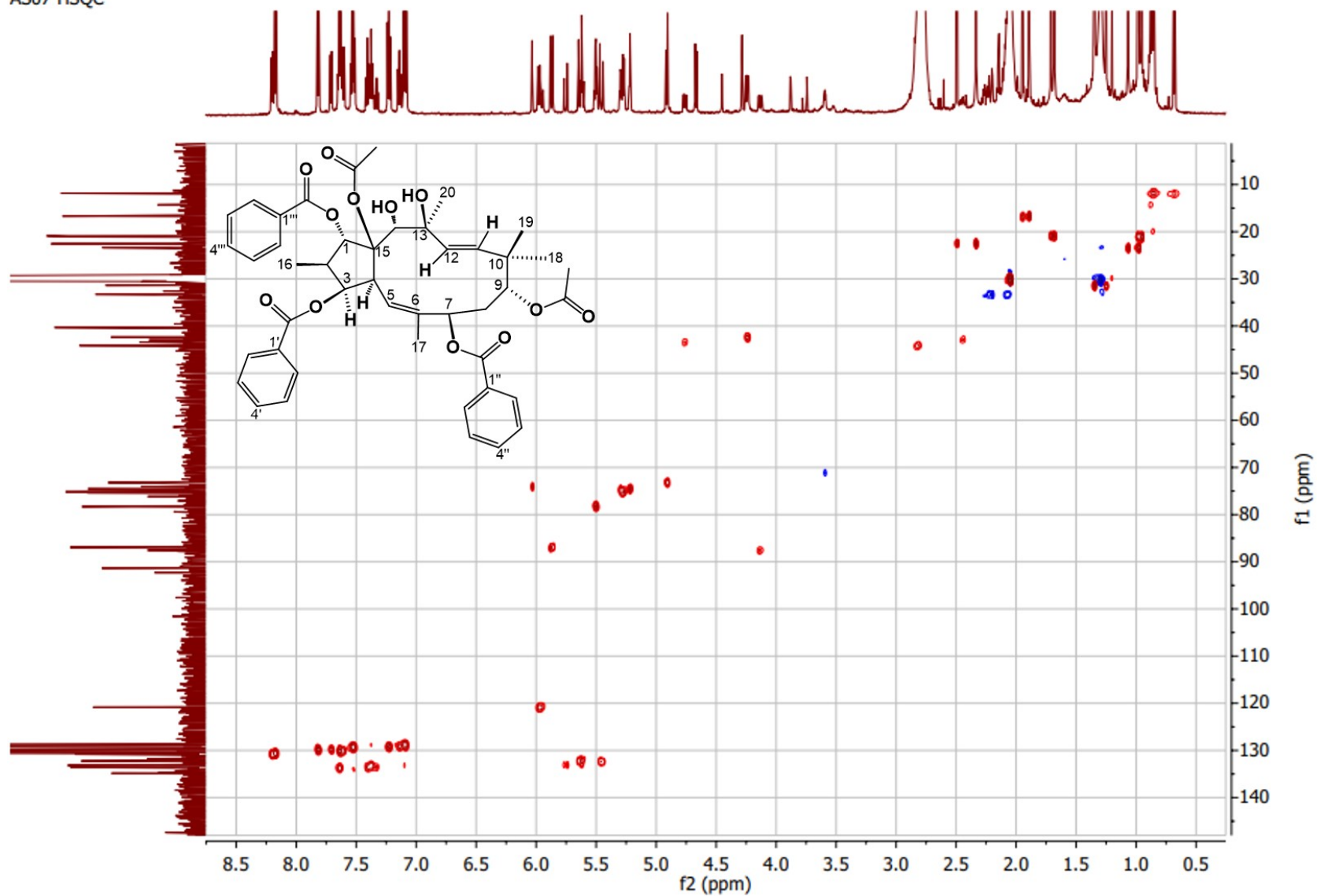


Figure S25. HSQC spectrum (sketched) of compound **P3** (Acetone- d_6)

AS07 HSQC

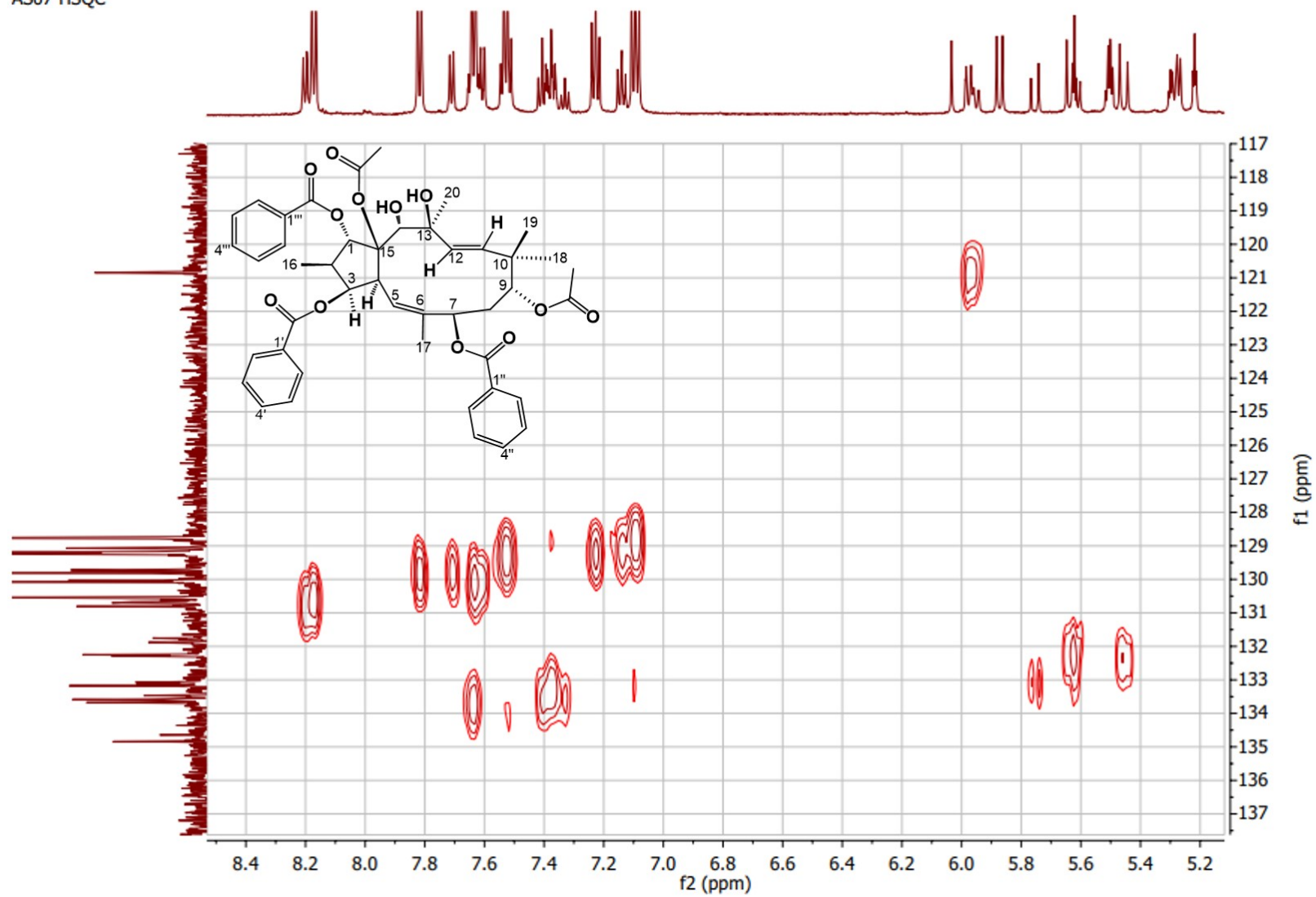


Figure S26. HMBC spectrum (total) of compound **P3** (Acetone- d_6)

AS07 HMBC

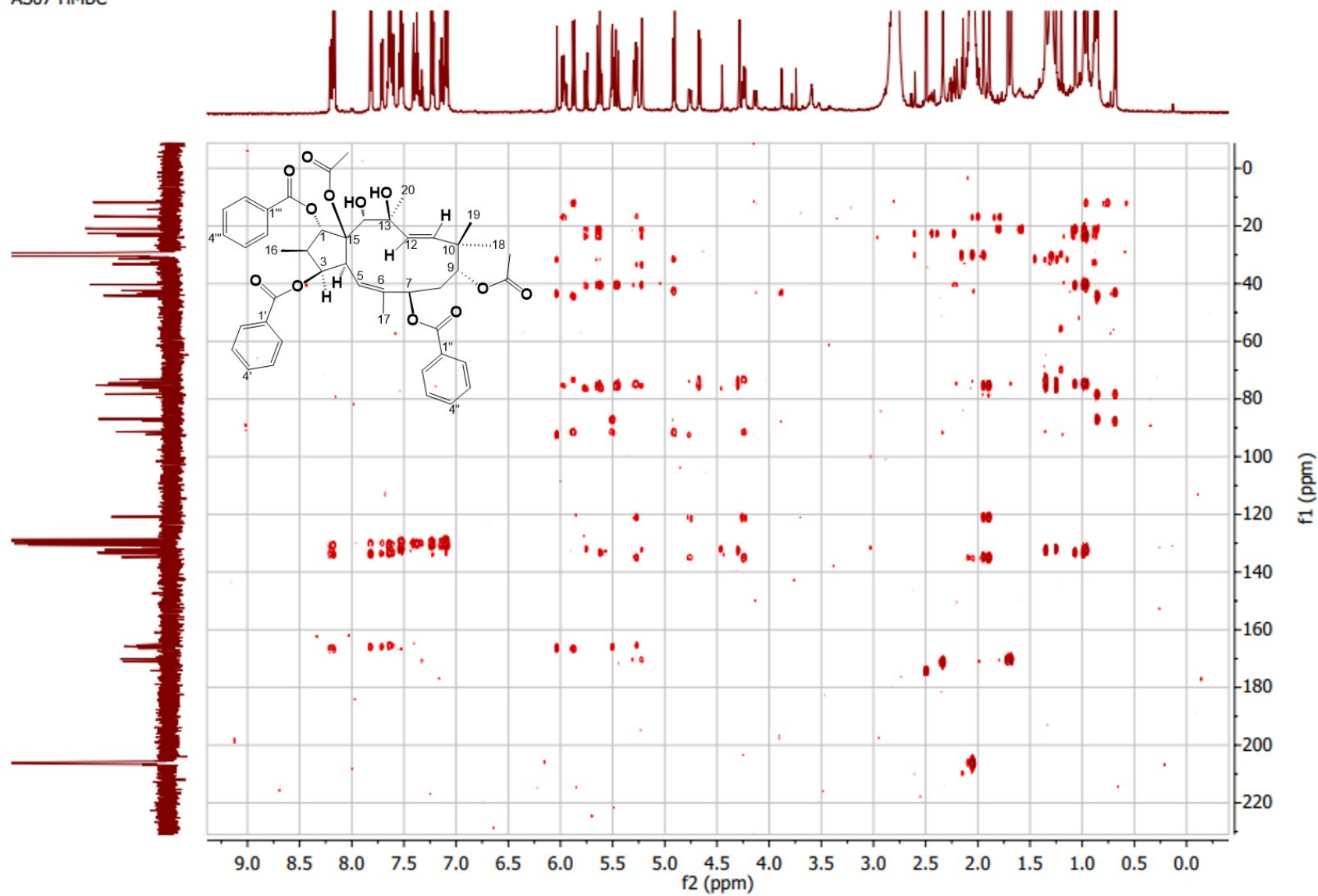


Figure S27. HMBC spectrum (sketched) of compound **P3** (Acetone- d_6)

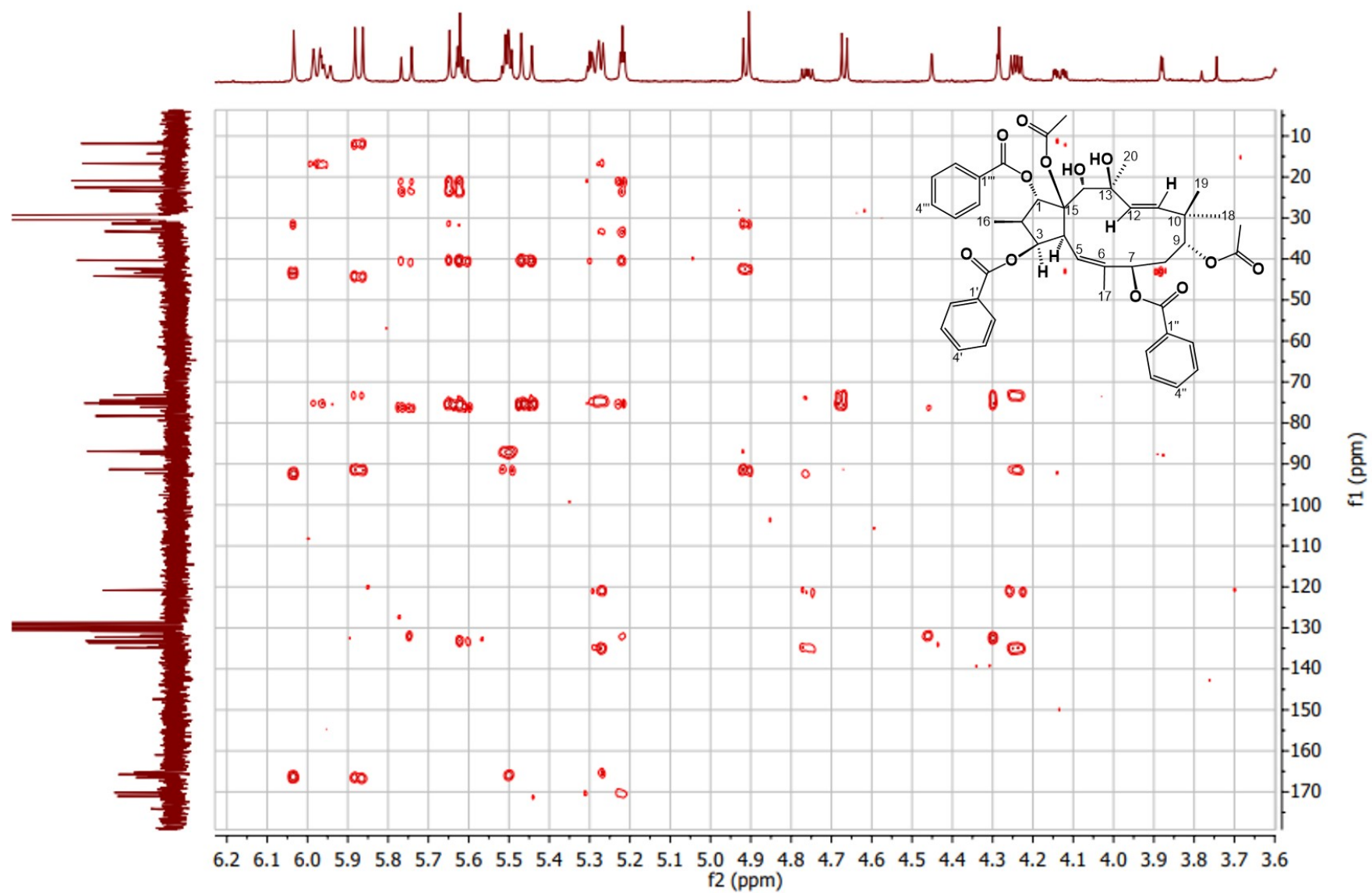


Figure S28. HMBC spectrum (sketched) of compound P3 (Acetone- d_6)

AS07 HMBC

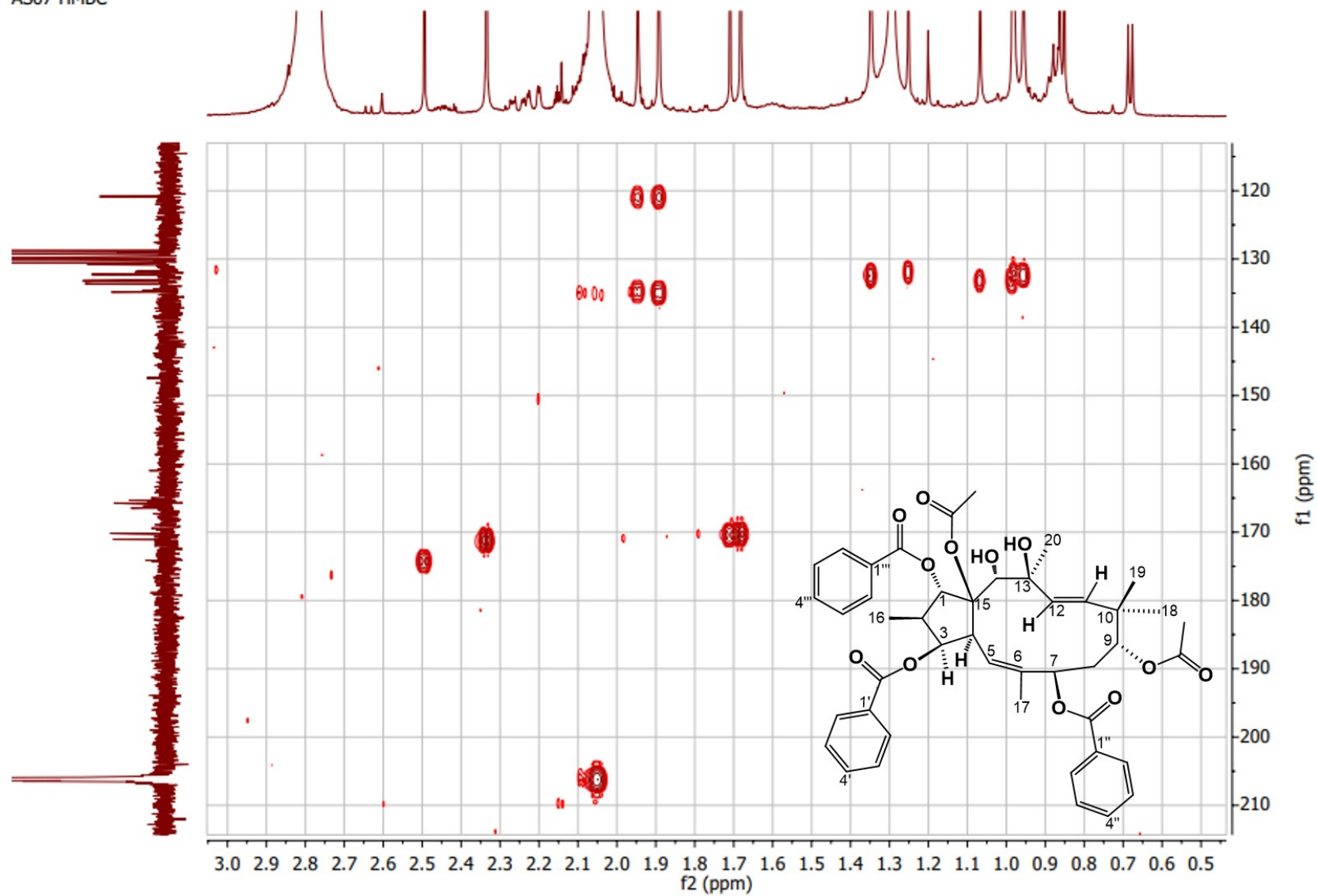


Figure S29. HMBC spectrum (sketched) of compound **P3** (Acetone- d_6)

AS07 HMBC

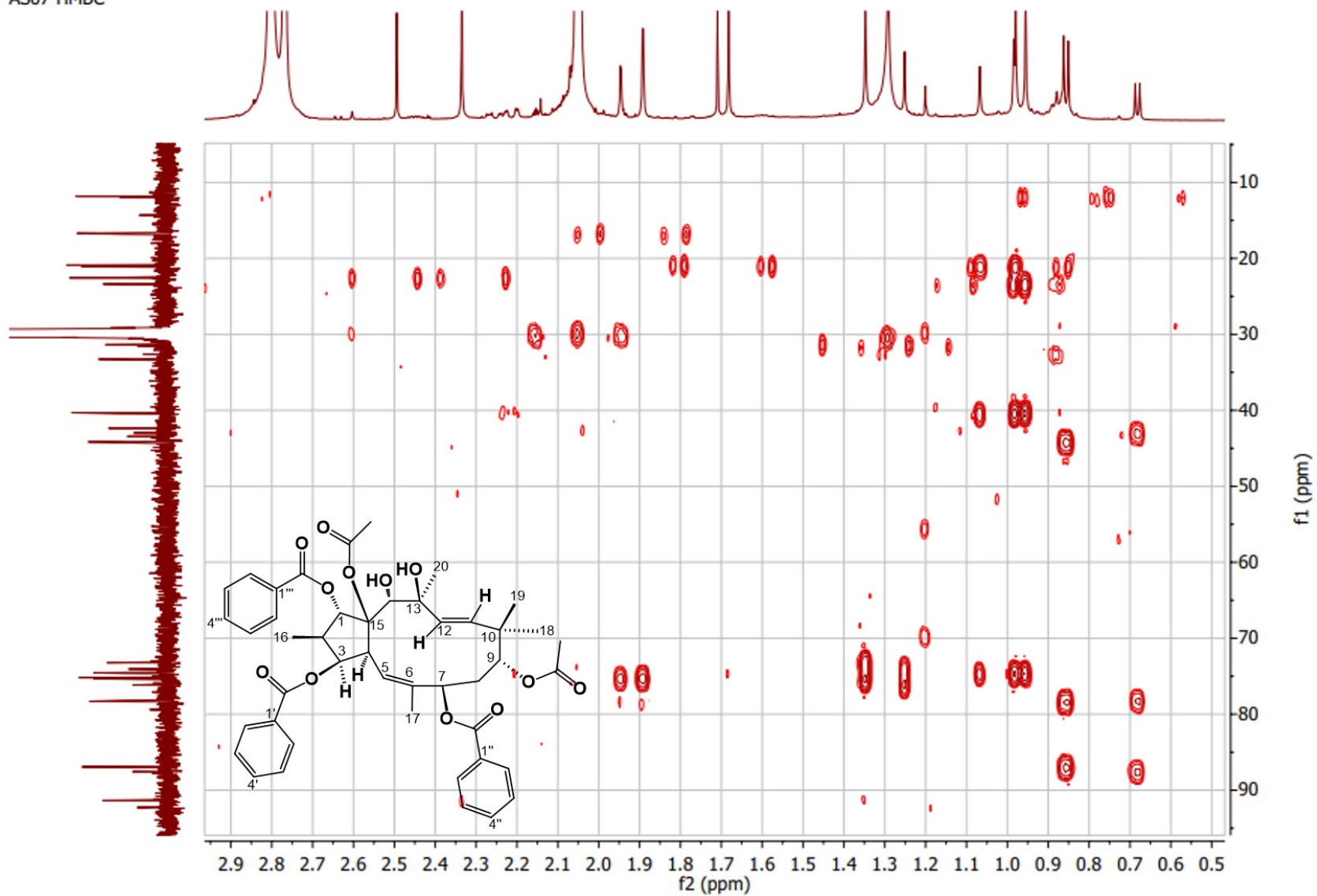


Figure S30. NOESY spectrum of compound **P3** (Acetone- d_6)

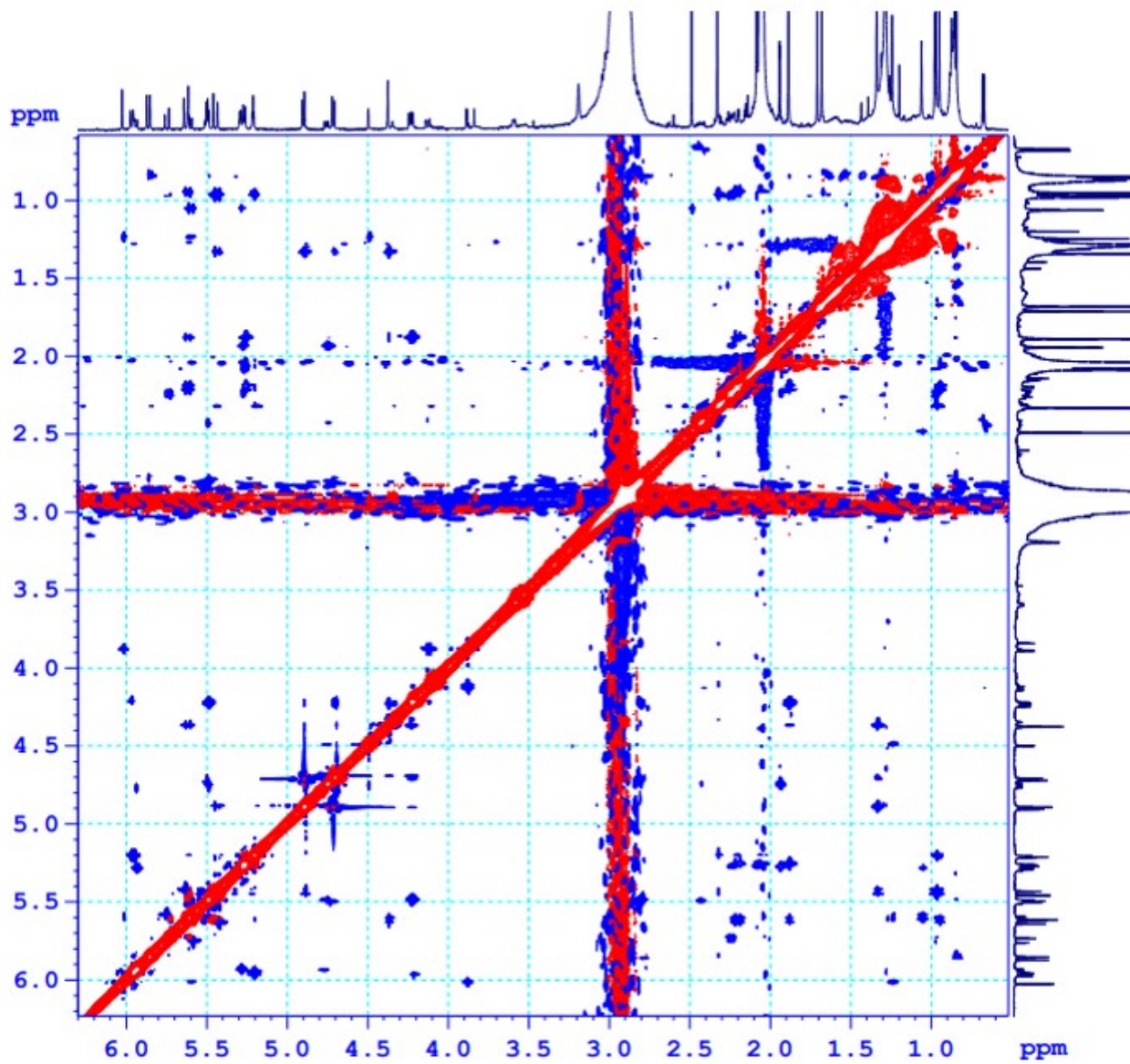


Figure S31. NOESY spectrum (sketched) of compound P3 (Acetone- d_6)

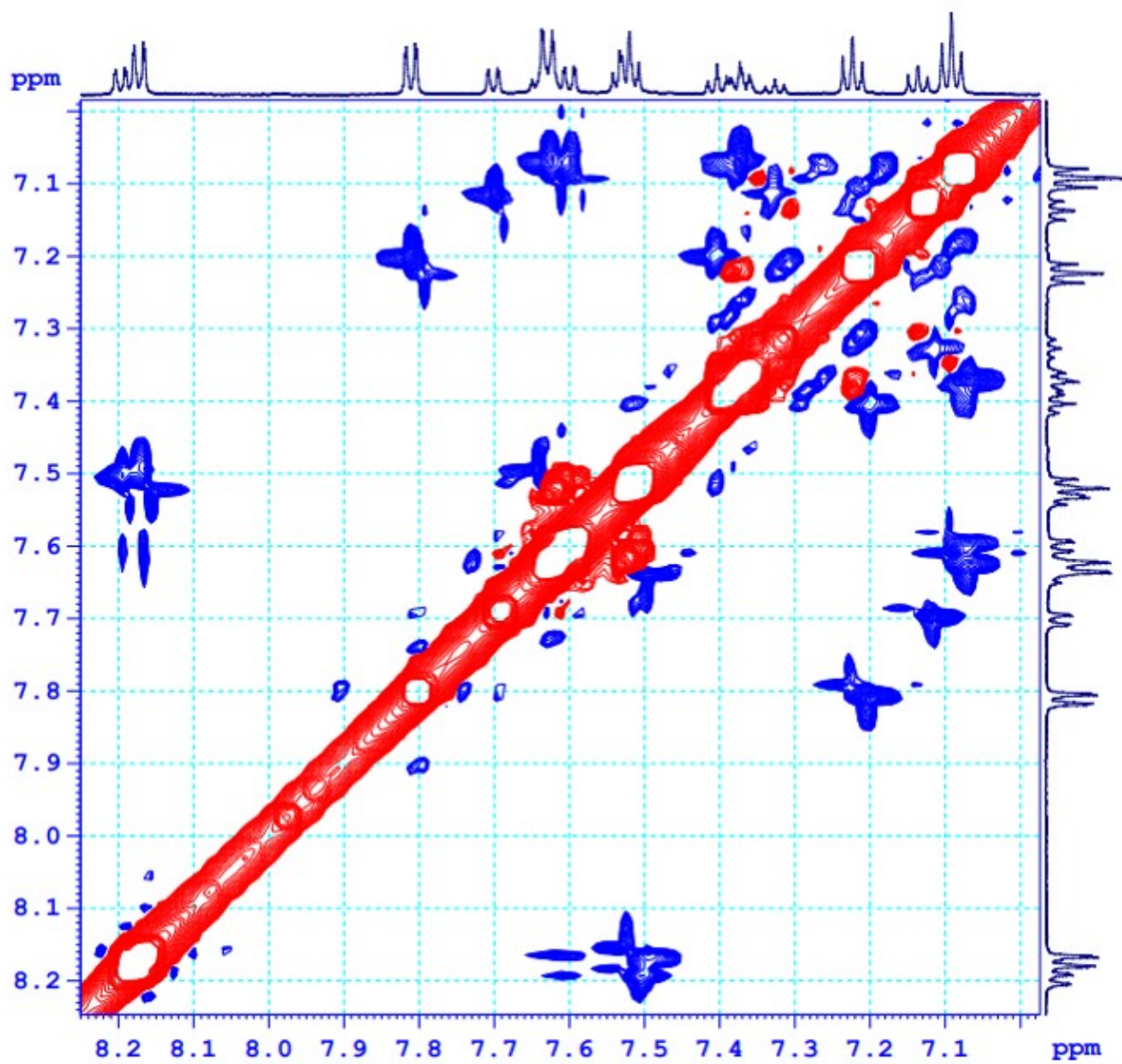


Figure S32. NOESY spectrum (sketched) of compound P3 (Acetone- d_6)

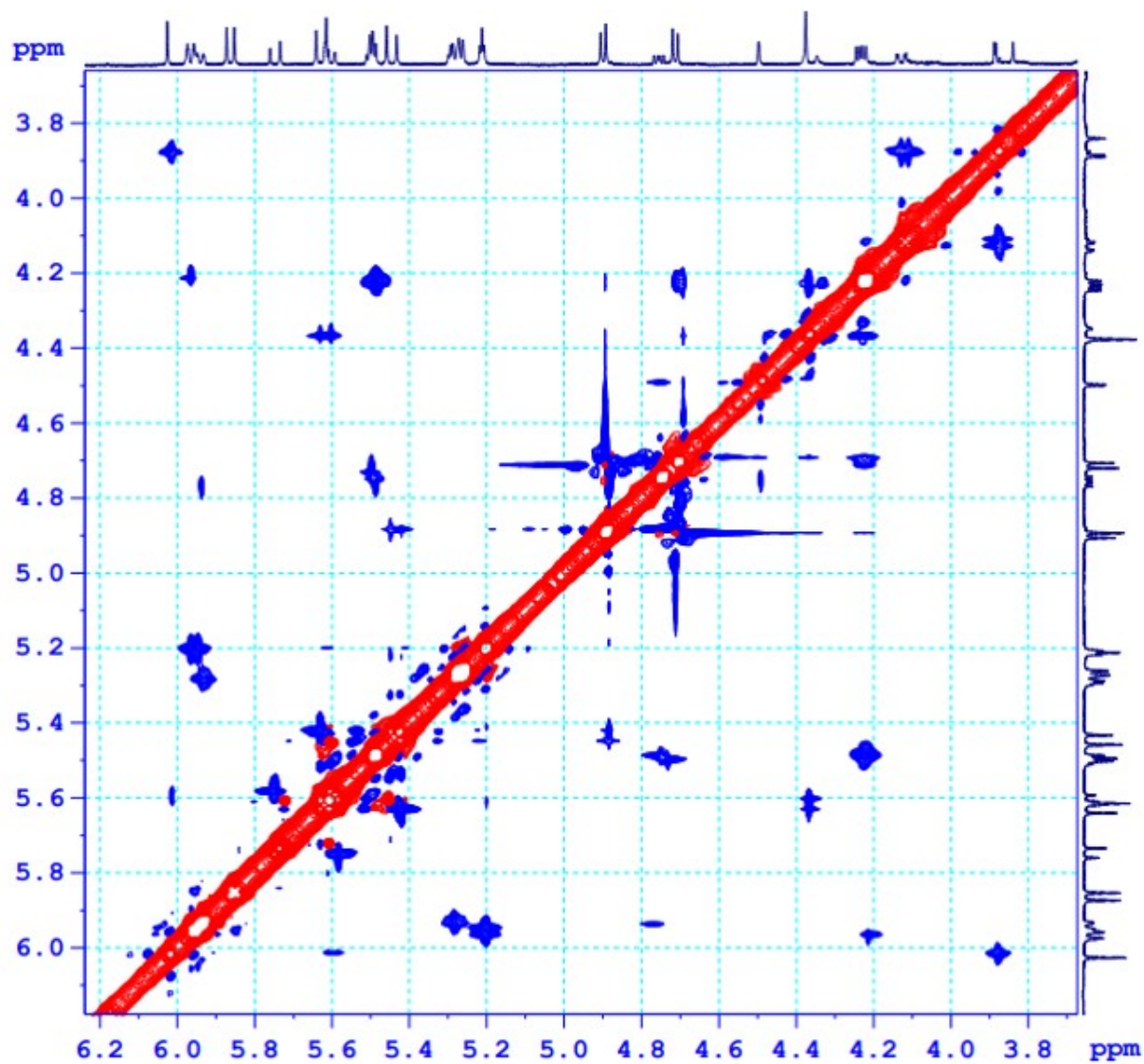


Figure S33. MS spectrum of compound **P3** (Acetone- d_6)

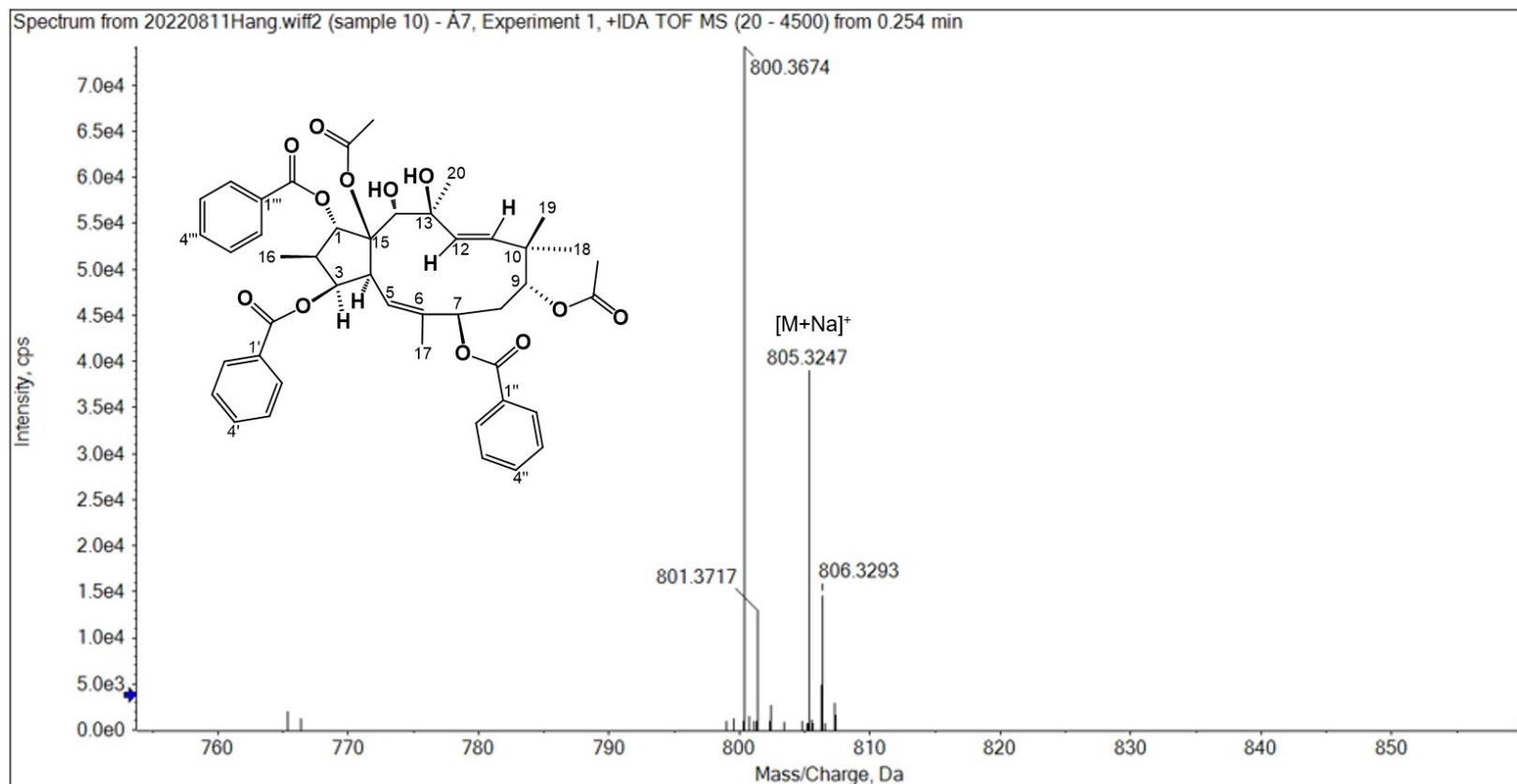


Figure S34. ¹H-NMR (600 MHz) spectrum of compound P4 (CDCl₃)

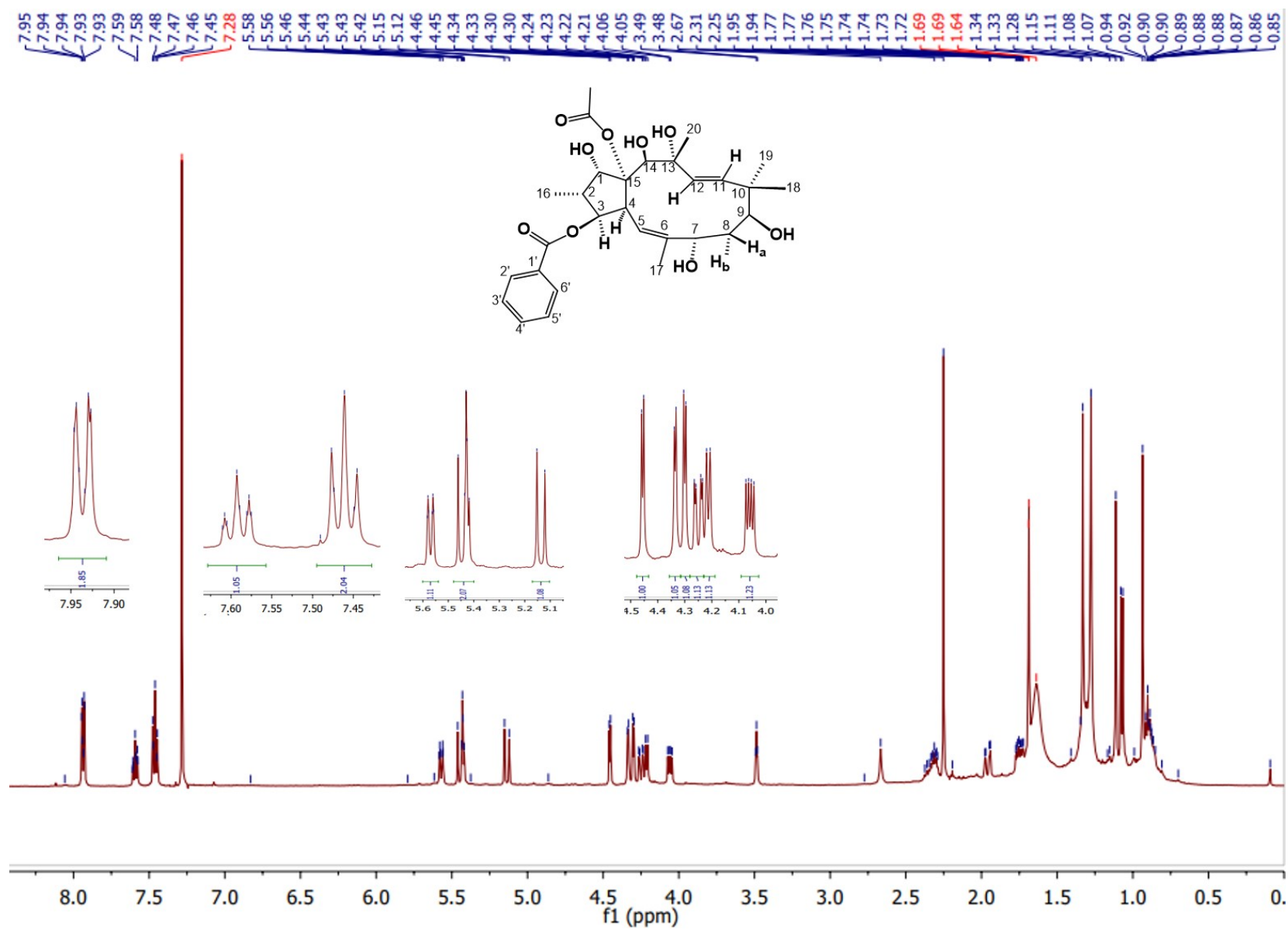


Figure S35. ^{13}C -NMR (125 MHz) spectrum of compound **P4** (CDCl_3)

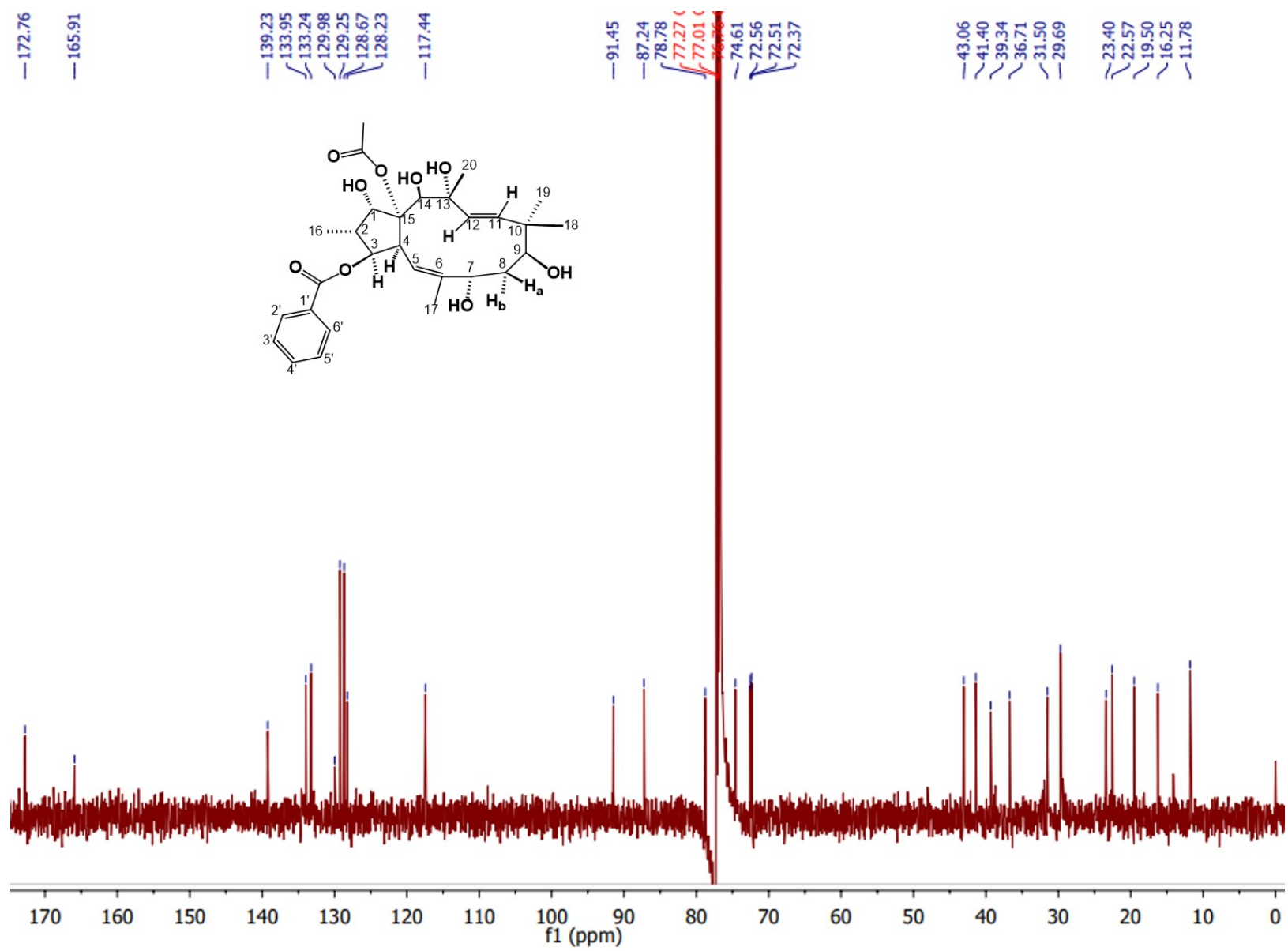


Figure S36. COSY spectrum of compound P4 (CDCl₃)

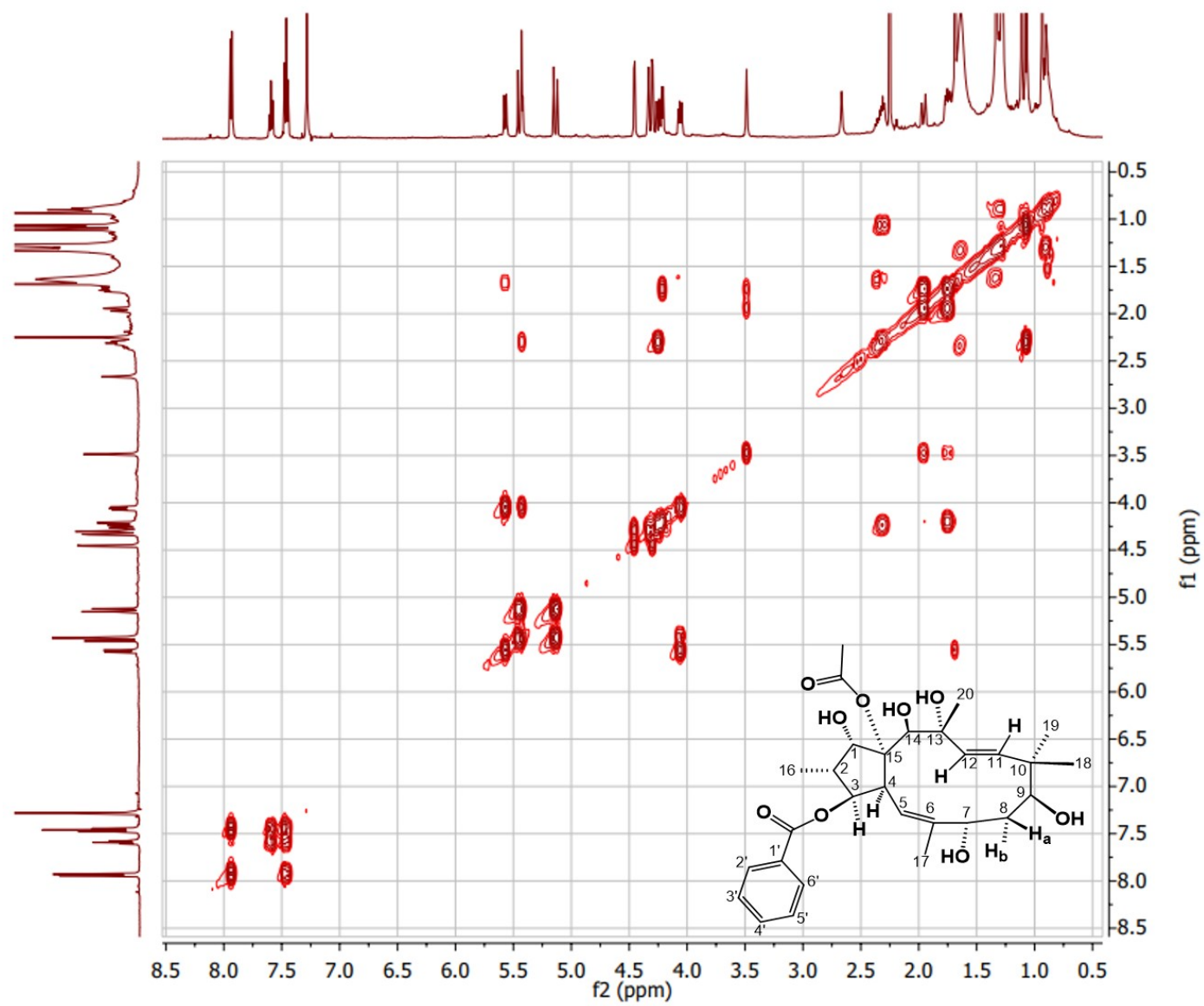


Figure S37. HSQC spectrum of compound **P4** (CDCl₃)

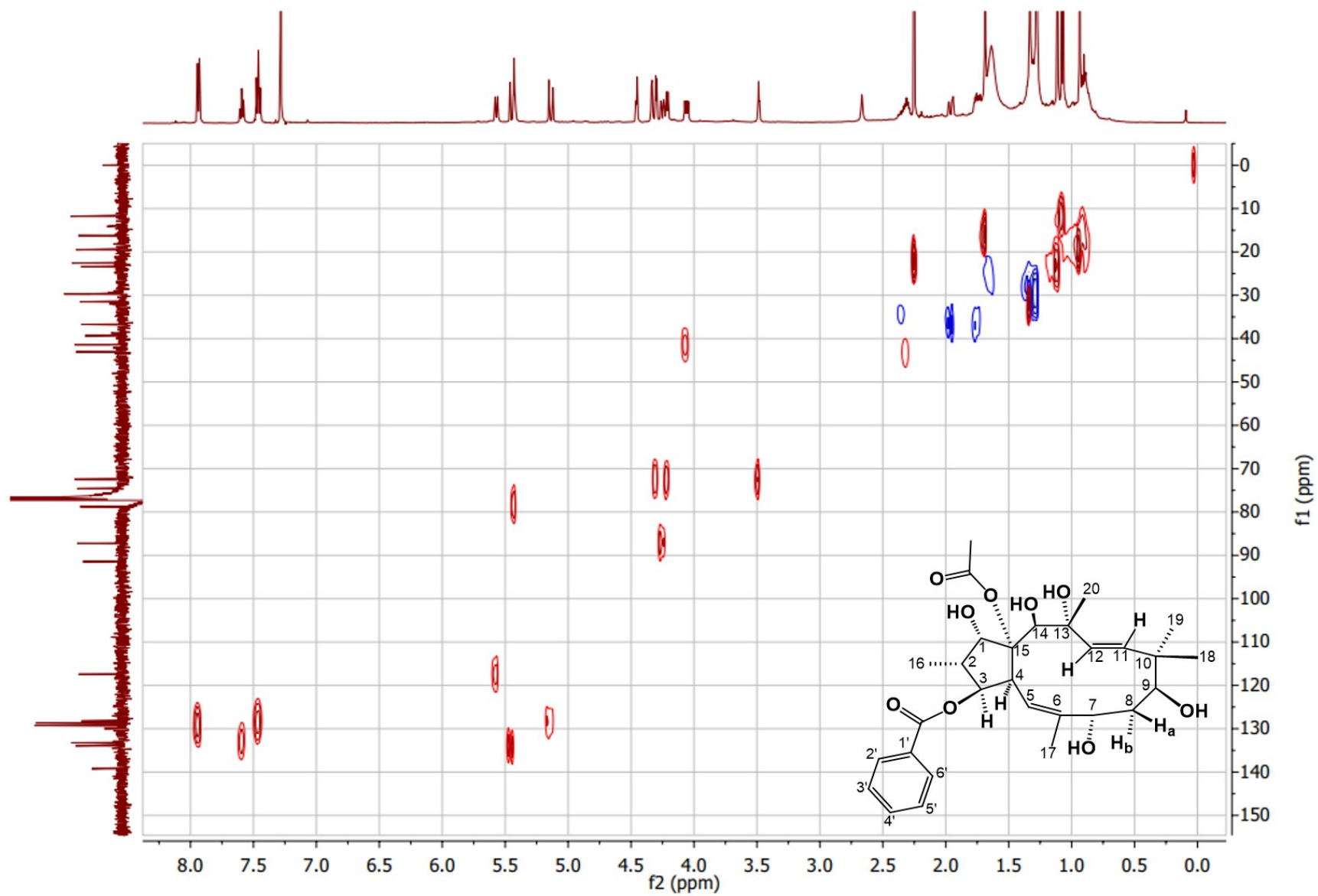


Figure S38. HMBC spectrum (total) of compound **P4** (CDCl₃)

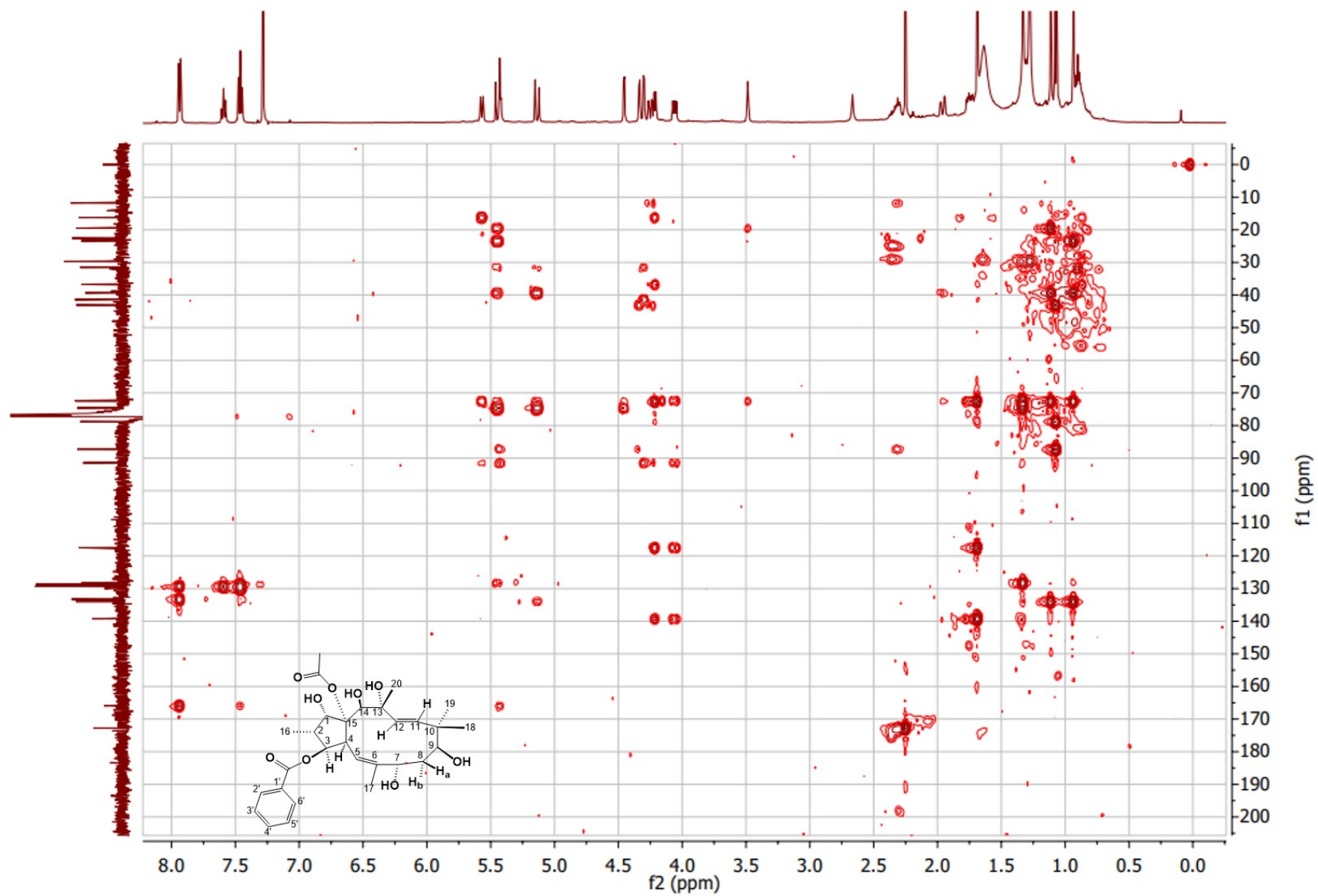


Figure S39. HMBC spectrum (sketched) of compound P4 (CDCl₃)

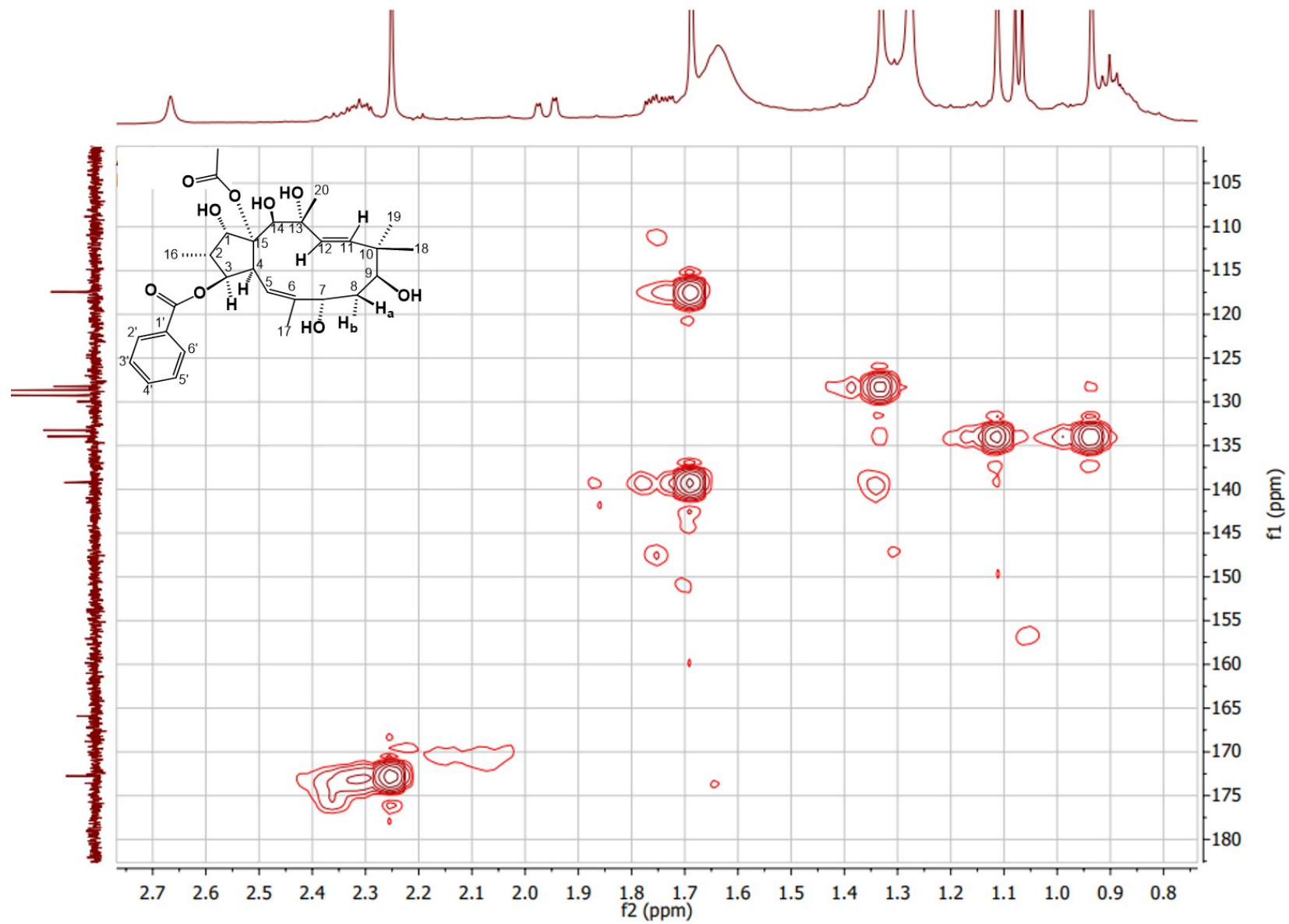


Figure S40. NOESY spectrum of compound **P4** (CDCl₃)

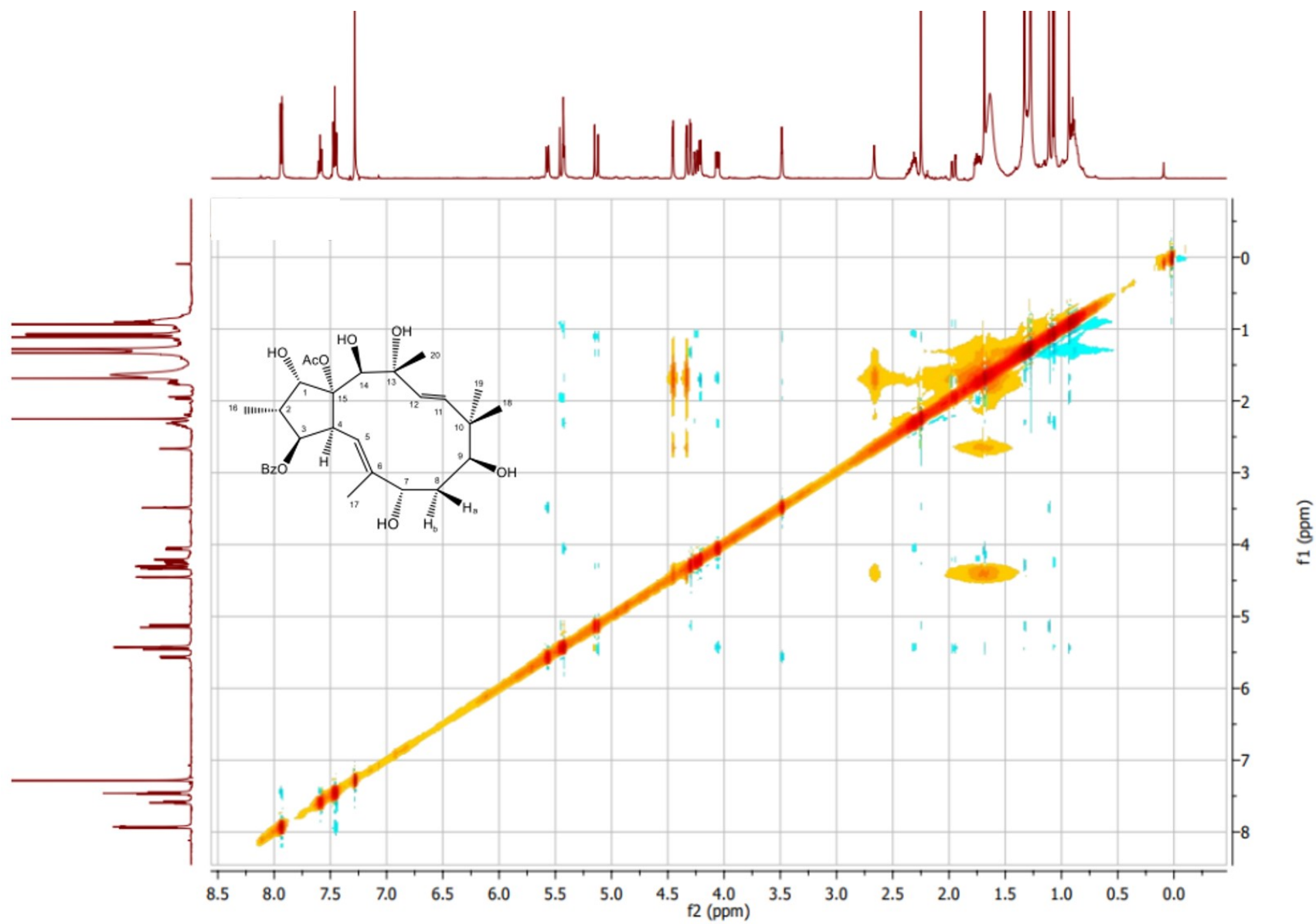
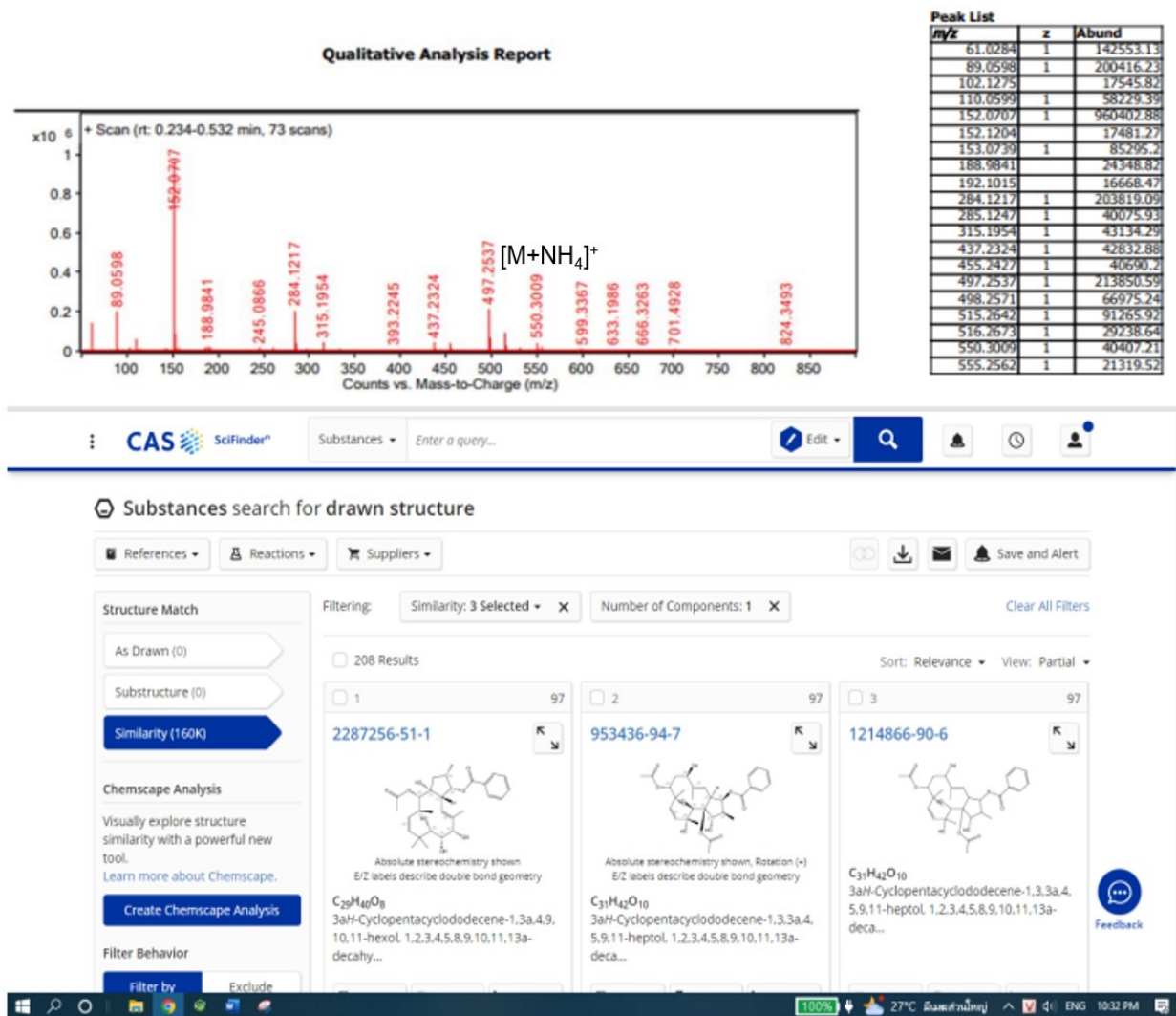


Figure S41. MS spectrum (CDCl₃) and structural novelty check for compound P4



Substances
10:31 PM

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

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

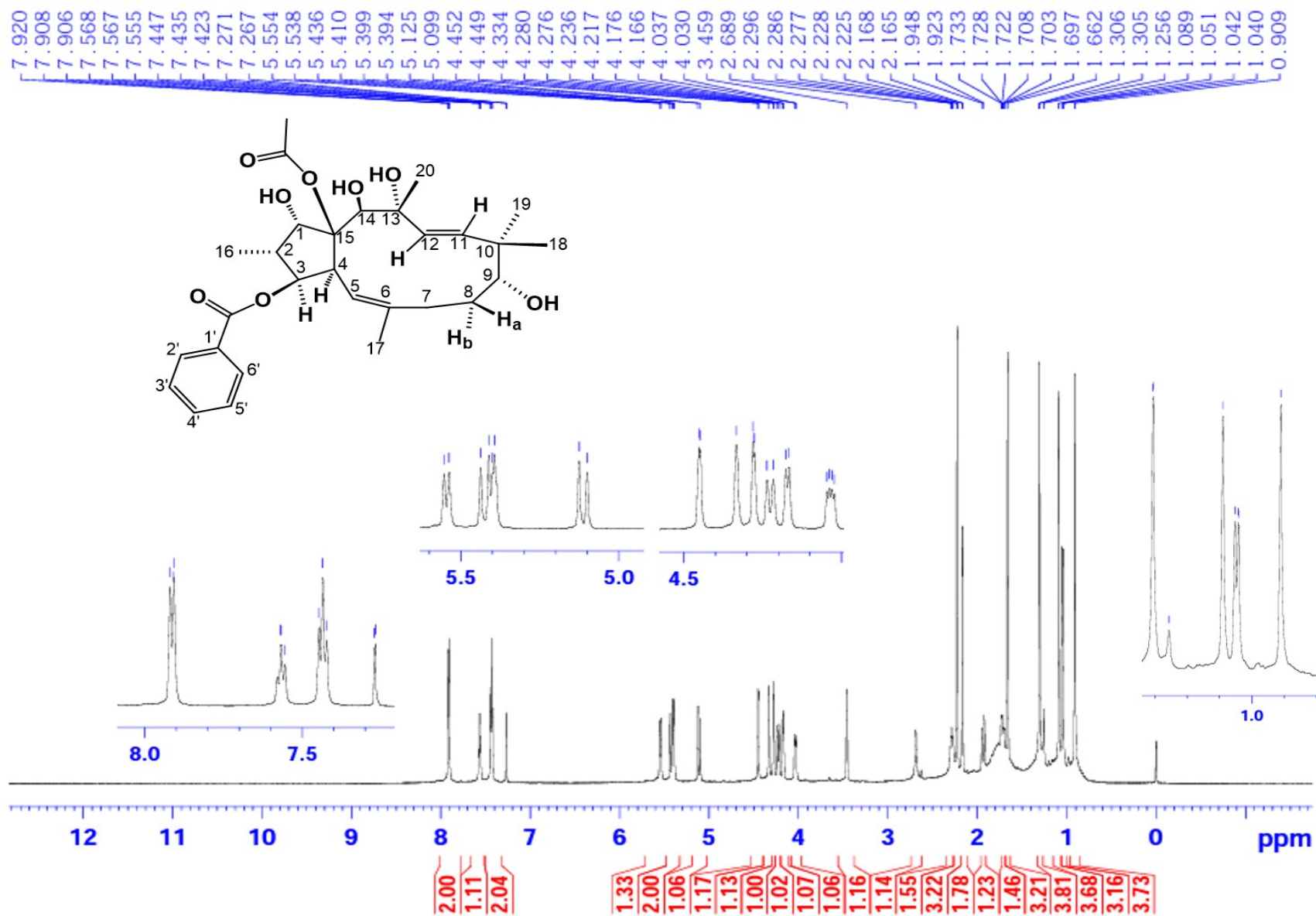


Figure S43. ^{13}C -NMR (125 MHz) spectrum of compound **P5** (CDCl_3)

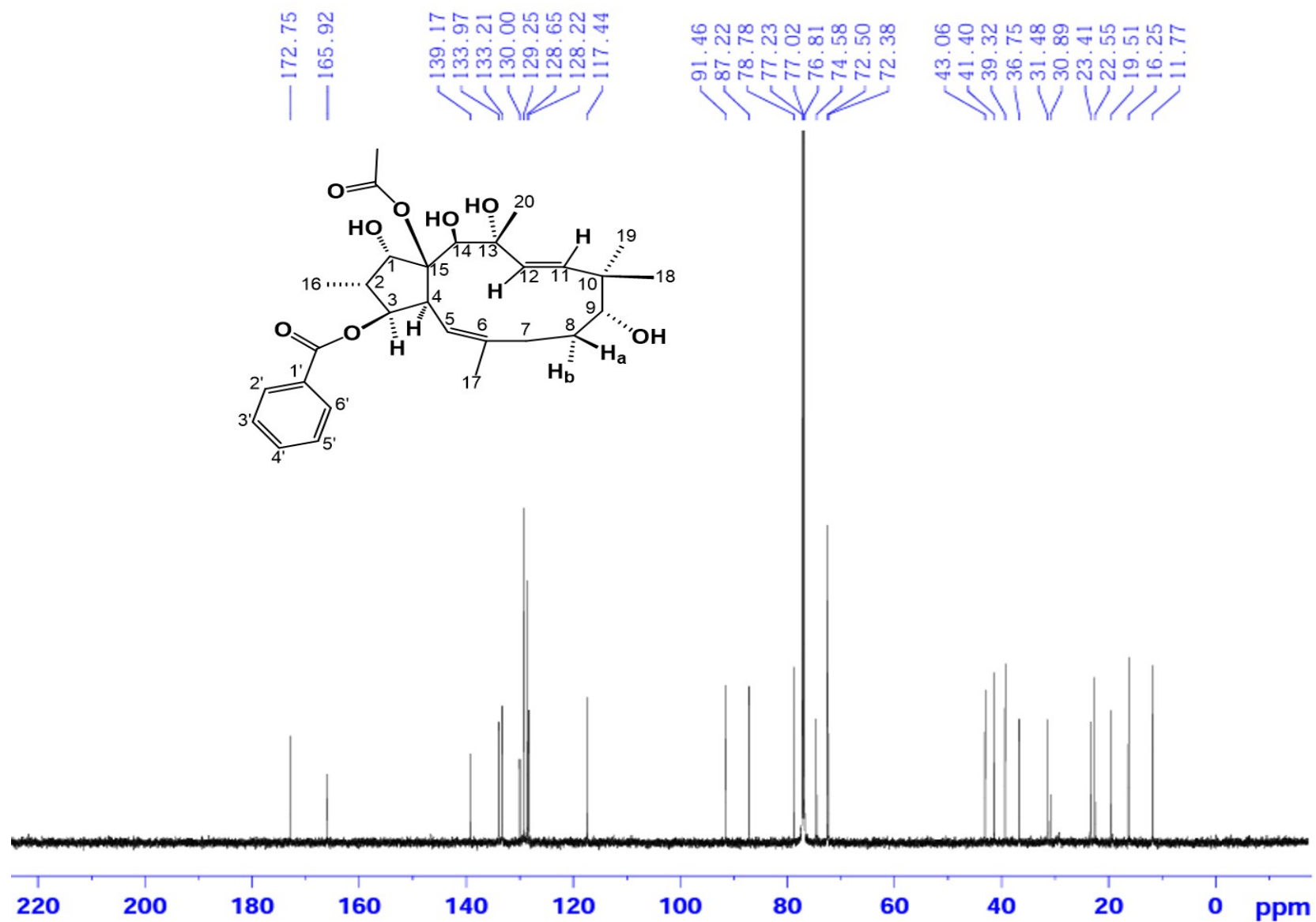


Figure S44. COSY spectrum of compound P5 (CDCl₃)

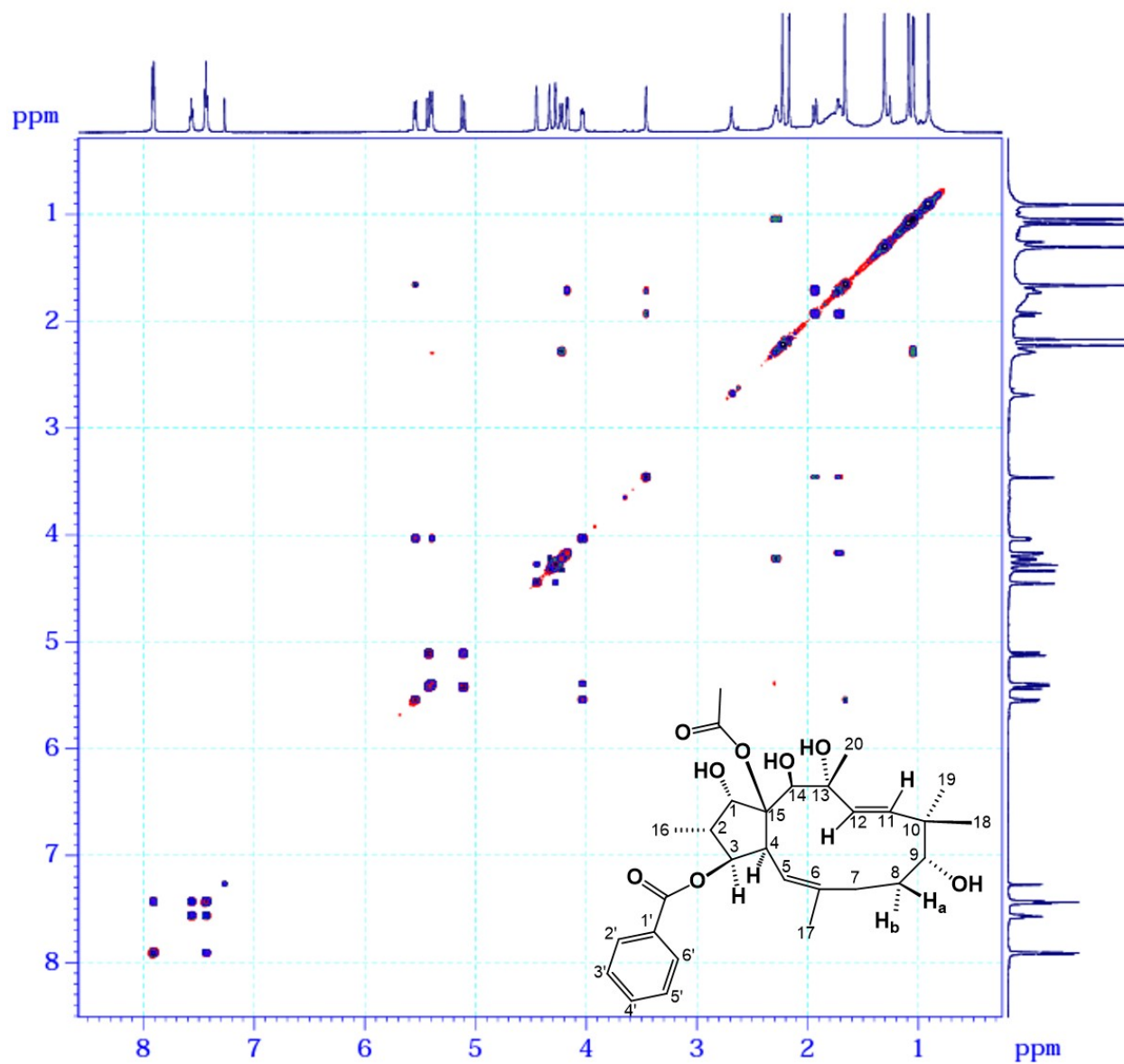


Figure S45. HSQC spectrum of compound P5 (CDCl₃)

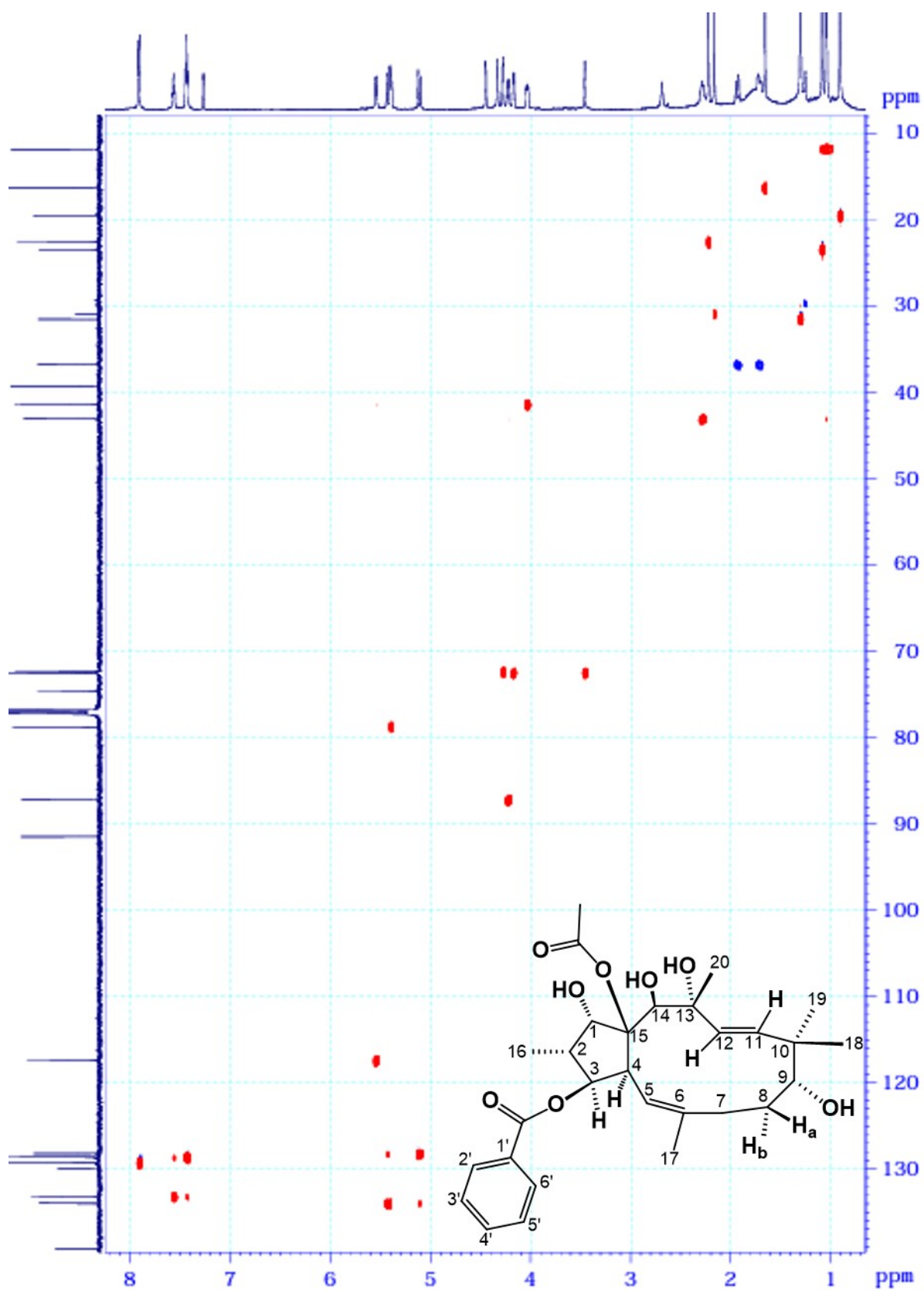


Figure S46. HMBC spectrum (total) of compound P5 (CDCl₃)

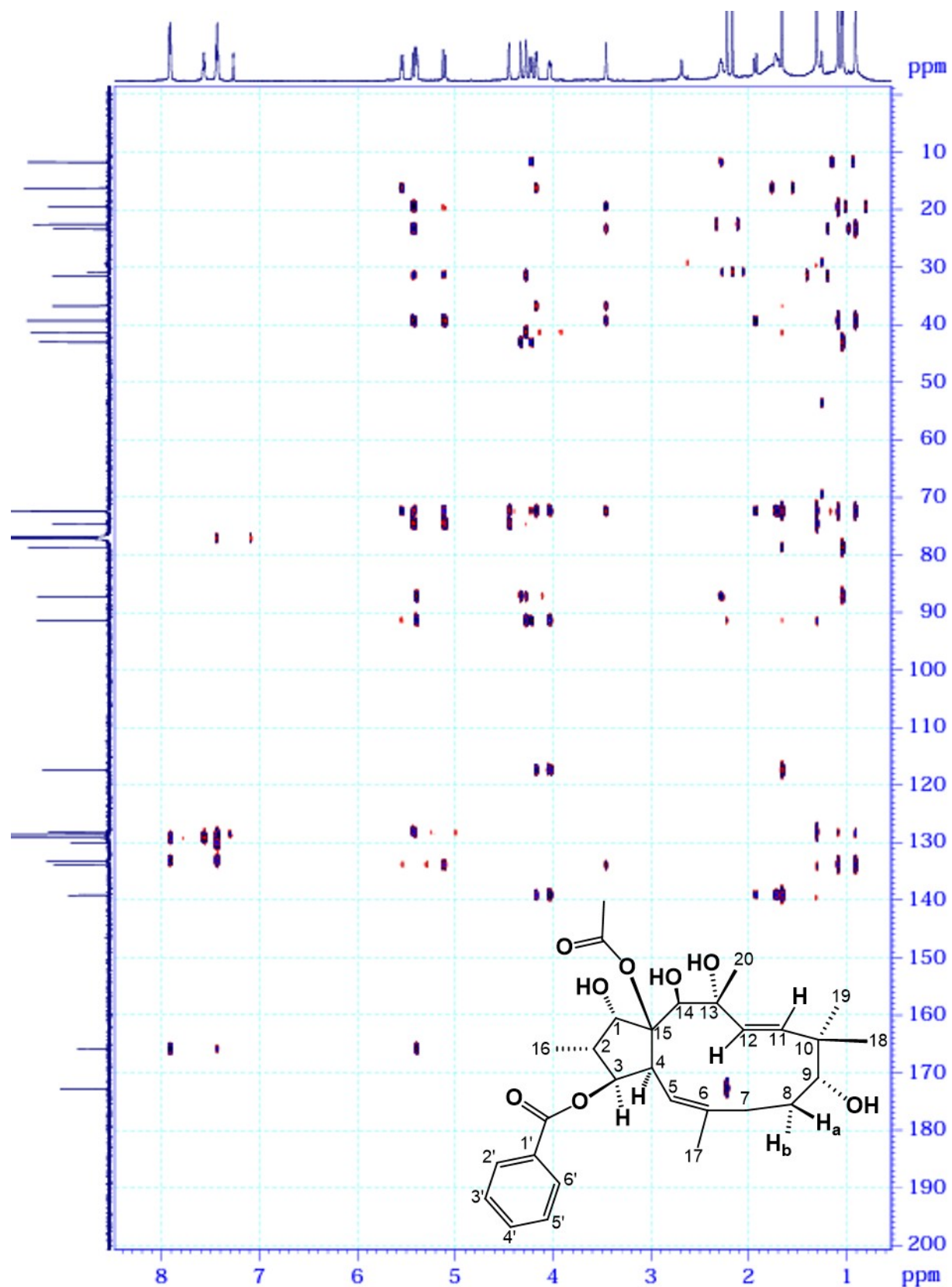


Figure S47. HMBC spectrum (sketched) of compound P5 (CDCl₃)

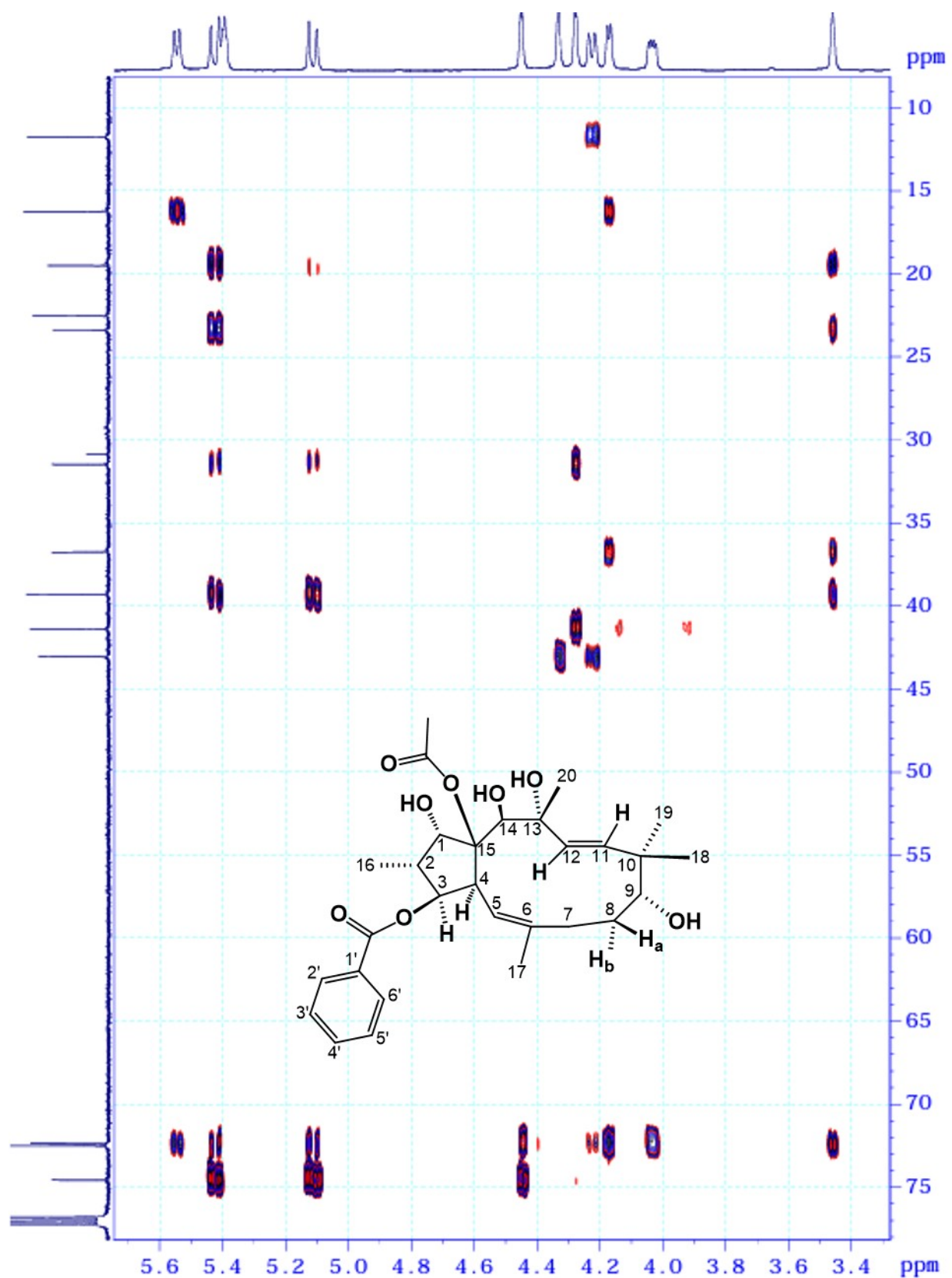


Figure S48. HMBC spectrum (sketched) of compound P5 (CDCl₃)

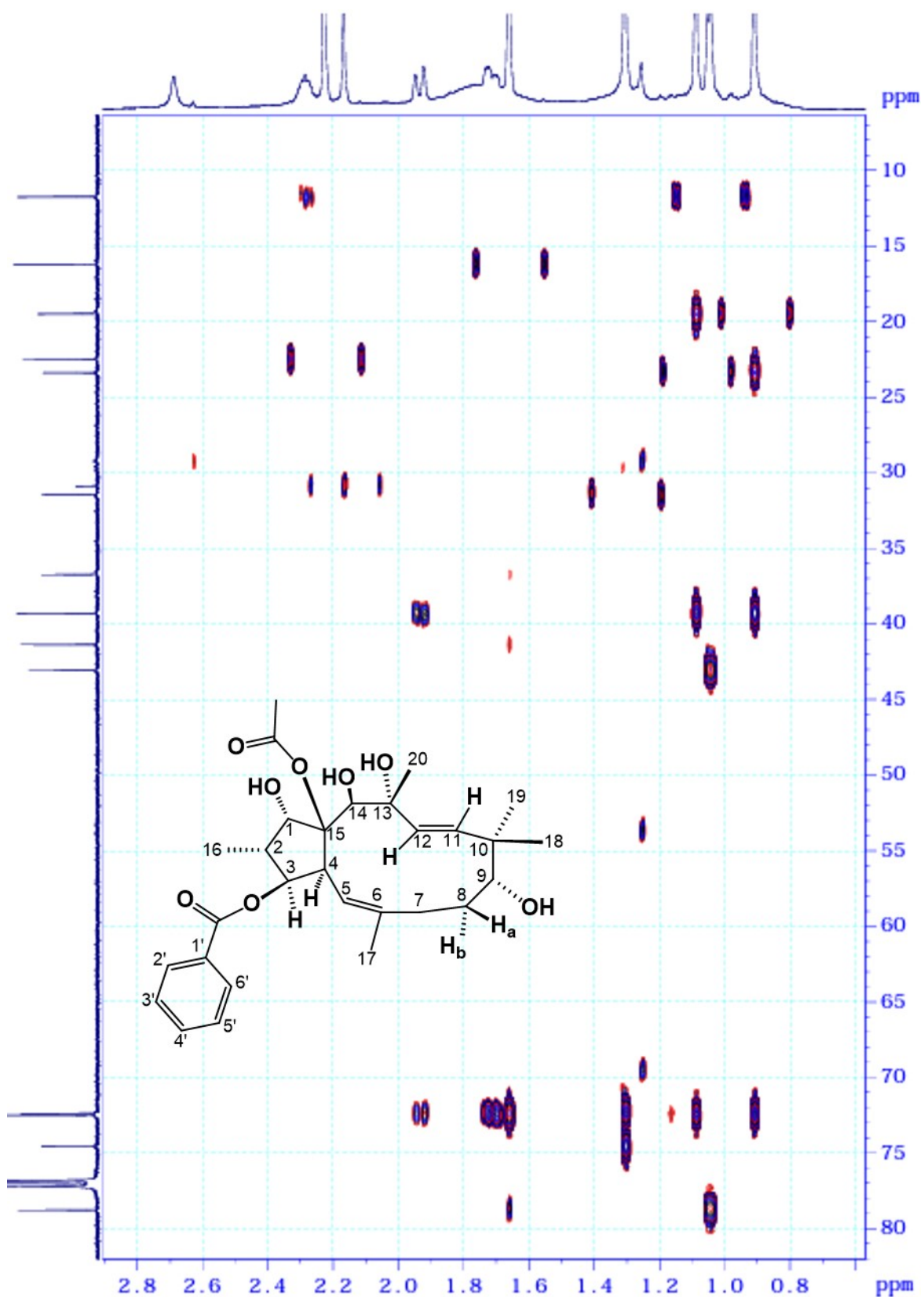


Figure S49. NOESY spectrum of compound P5 (CDCl₃)

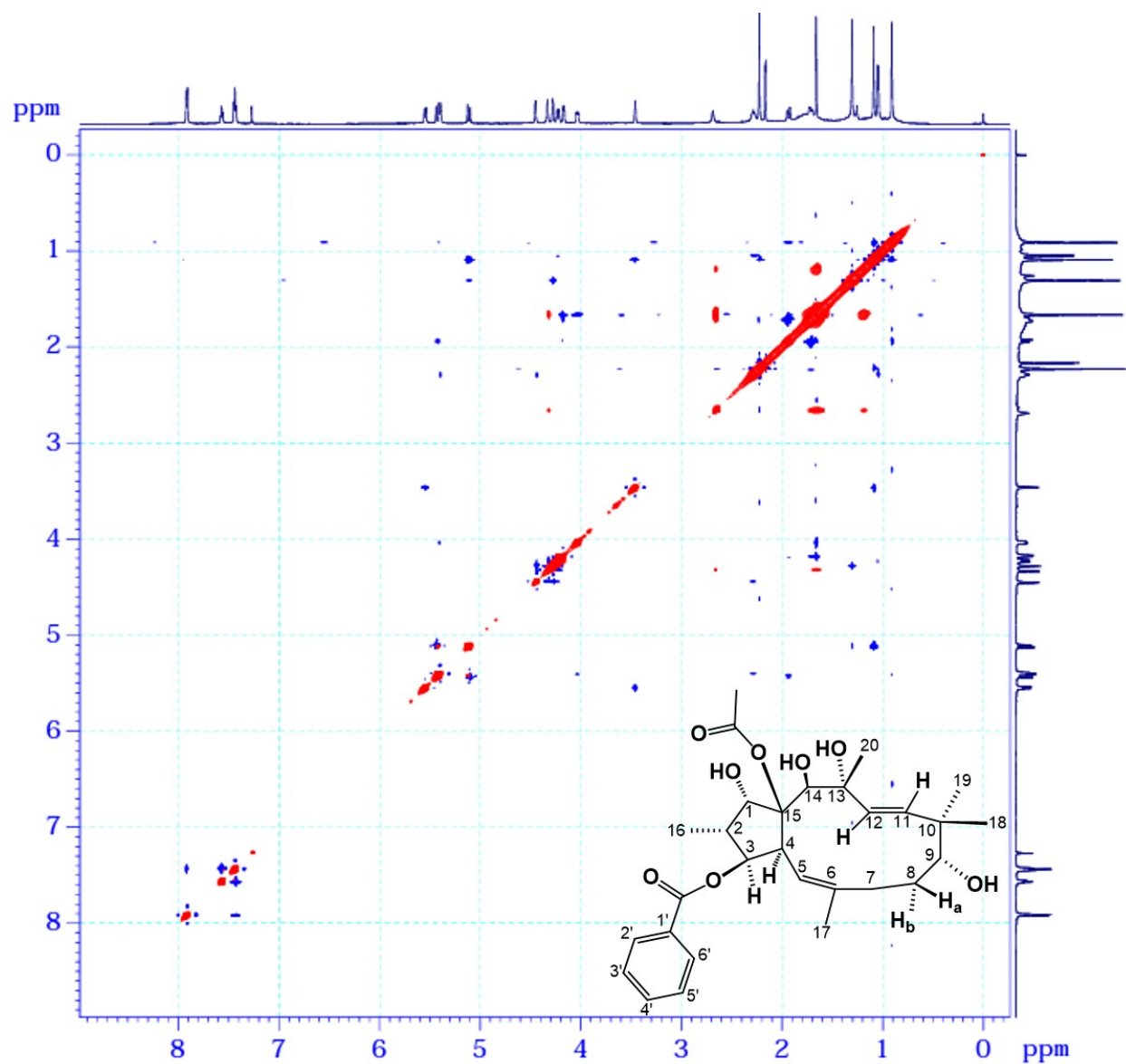


Figure S50. MS spectrum of compound P5 (CDCl_3)



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

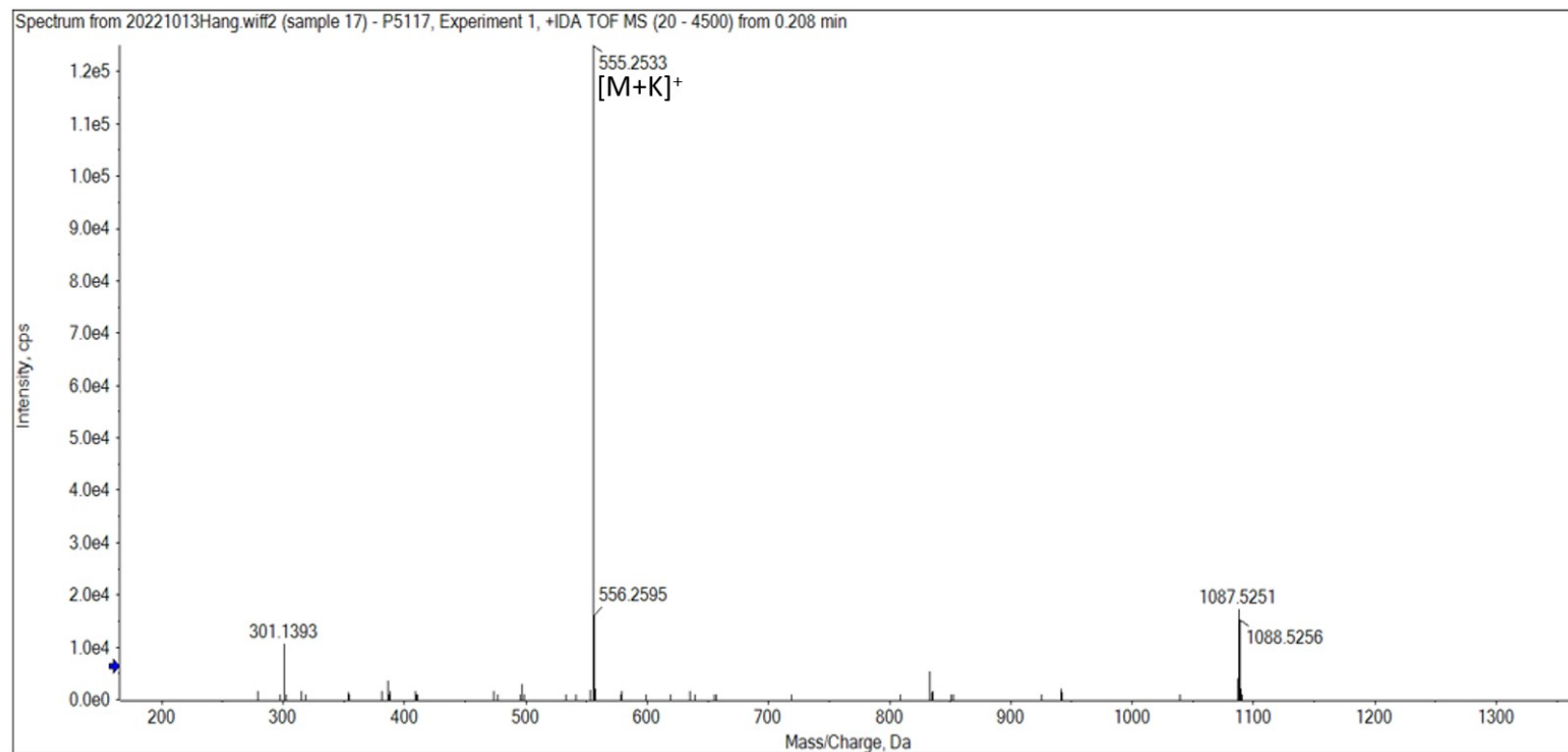


Figure S51. Structural novelty check for compound P5

Substances search for drawn structure

References Reactions Suppliers

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

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

Filter Behavior: Filter by Exclude

Filtering: Similarity: 3 Selected, Number of Components: 1

181 Results

Sort: Relevance, View: Partial

Result ID	Chemical Structure	Description
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1946844-10-5		Absolute stereochemistry shown, Rotation (i) E/Z labels describe double bond geometry
1016572-85-2		Absolute stereochemistry shown, Rotation (i) E/Z labels describe double bond geometry

November 15, 2022

Substances 10:25 PM

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

Rerun Search

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