

Biologically active compounds in *Stizolophus balsamita* inflorescences: isolation, phytochemical characterization and effects on the skin biophysical parameters

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Supplementary material

List of supporting information

Compound **1** (izospiciformin).

Compound **2**(stizolin).

Compound **3**(stizolicin).

Compound **4**(quercetin).

Compound **5** (kaempferol).

Compound **6** (rhamnetin).

Compound **7**(taxifolin).

Compound **8** (kaempferol 3-*O*- α -rhamnoside).

Compound **9**(ajugasterone C).

Compound **10**(arbutin).

Compound **11** (protocatechuic acid methyl ester).

List of spectra:

Figure S1. ¹H NMR spectrum (600 MHz, CD₃OD) of compound **4**.

Figure S2. ¹H NMR spectrum (600 MHz, CD₃OD) of compound **5**.

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Figure S5. ¹³C NMR spectrum (150 MHz, CD₃OD) of compound **7**.

Figure S6. HH-COSY spectrum (600 MHz, CD₃OD) of compound **7**.

Figure S7. HSQC spectrum (600/150 MHz, CD₃OD) of compound **7**.

Figure S8. HMBC spectrum (600/150 MHz, CD₃OD) of compound **7**.

Figure S9. NOESY spectrum (600 MHz, CD₃OD) of compound **7**.

Figure S10. ¹H NMR spectrum (600 MHz, CD₃OD) of a mixture of compounds **8** and **9**. Only signals of compound **8** are labeled.

Figure S11. ¹³C NMR spectrum (150 MHz, CD₃OD) of a mixture of compounds **8** and **9**.

Figure S12. ^{13}C NMR spectrum (150 MHz, CD_3OD) of a mixture of compounds **8** and **9**. Only signals of compound **8** are labeled.

Figure S13. HH-COSY spectrum (600 MHz, CD_3OD) of a mixture of compounds **8** and **9**. Only signals of compound **8** are labeled.

Figure S14. HSQC spectrum (600/150 MHz, CD_3OD) of a mixture of compounds **8** and **9**. Only signals of compound **8** are labeled.

Figure S15. HMBC spectrum (600/150 MHz, CD_3OD) of a mixture of compounds **8** and **9**. Only signals of compound **8** are labeled.

Figure S16. NOESY spectrum (600 MHz, CD_3OD) of a mixture of compounds **8** and **9**.

Figure S17. ^1H NMR spectrum (600 MHz, CD_3OD) of a mixture of compounds **7**, **10** and **11**.

Figure S18. ^1H NMR spectrum (600 MHz, CD_3OD) of a mixture of compounds **7**, **10** and **11**. Only signals of compound **11** are labeled.

Figure S19. ^1H NMR spectrum (600 MHz, CD_3OD) of a mixture of compounds **7**, **10** and **11**. Only signals of compound **10** are labeled.

Figure S20. ^1H NMR spectrum (600 MHz, CD_3OD) of a mixture of compounds **7**, **10** and **11**. Only signals of compound **7** are labeled.

Figure S21. ^{13}C NMR spectrum (150 MHz, CD_3OD) of a mixture of compounds **7**, **10** and **11**.

Figure S22. HH-COSY spectrum (600 MHz, CD_3OD) of a mixture of compounds **7**, **10** and **11**.

Figure S23. HSQC spectrum (600/150 MHz, CD_3OD) of a mixture of compounds **7**, **10** and **11**.

Figure S24. HMBC spectrum (600/150 MHz, CD_3OD) of a mixture of compounds **7**, **10** and **11**. The signals of compound **7** are labeled.

Figure S25. ^1H NMR spectrum (600 MHz, CD_3OD) of arbutin from *Serratulaquinquefolia*.

Figure S26. ^{13}C NMR spectrum (150 MHz, CD_3OD) of arbutin from *Serratulaquinquefolia*.

Figure S27. HH-COSY spectrum (600 MHz, CD_3OD) of arbutin from *Serratulaquinquefolia*.

Figure S28. HSQC spectrum (600/150 MHz, CD_3OD) of arbutin from *Serratulaquinquefolia*.

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Table S1.

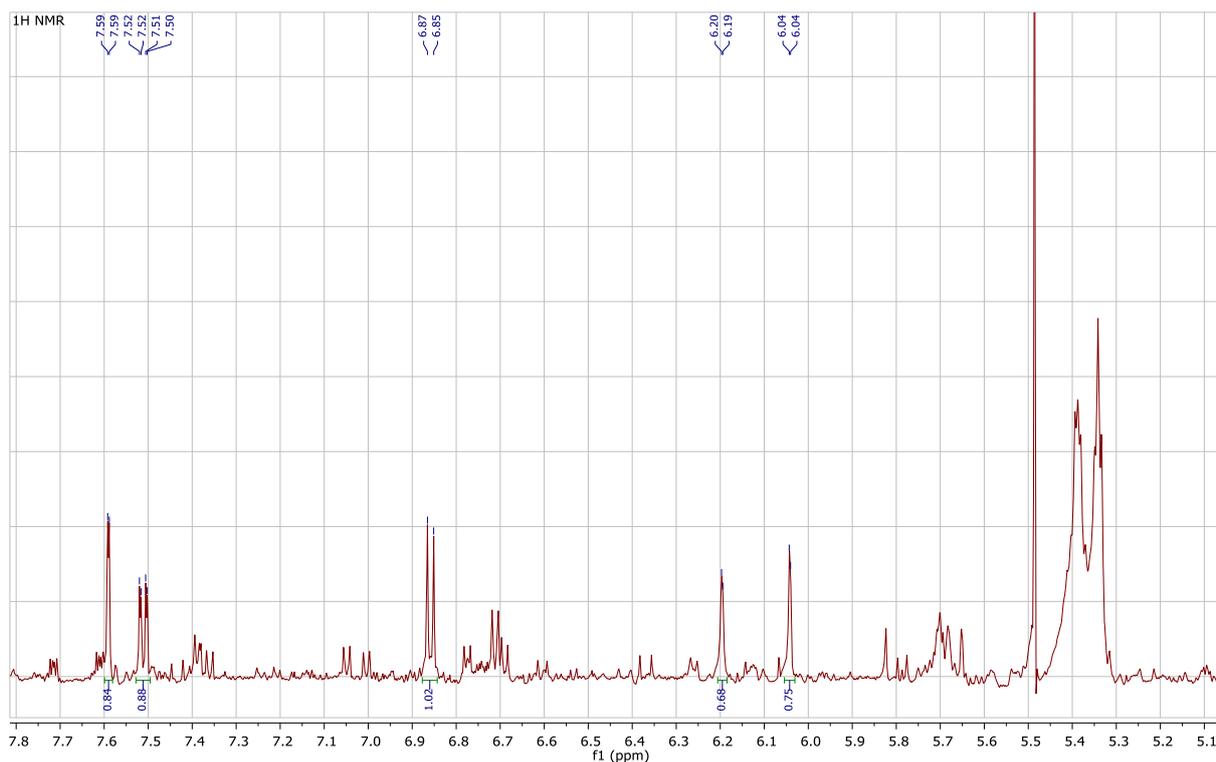


Figure S1. ¹H NMR spectrum (600 MHz, CD₃OD) of compound 4.

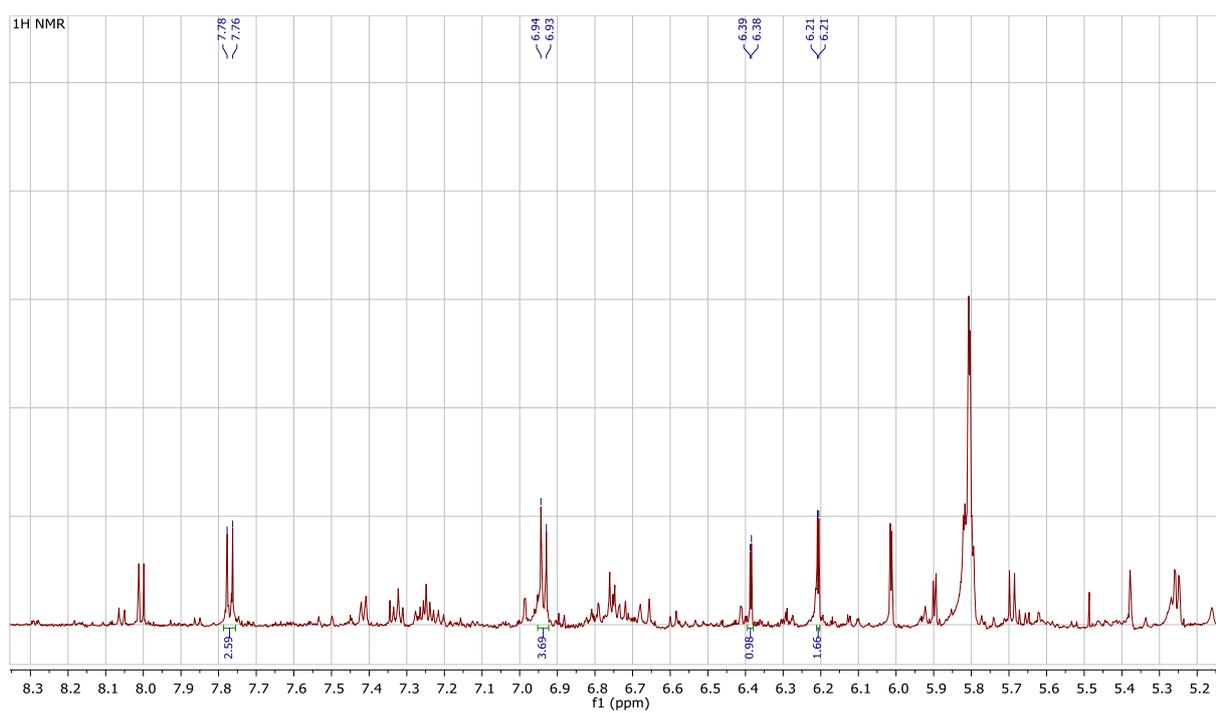


Figure S2. ¹H NMR spectrum (600 MHz, CD₃OD) of compound 5.

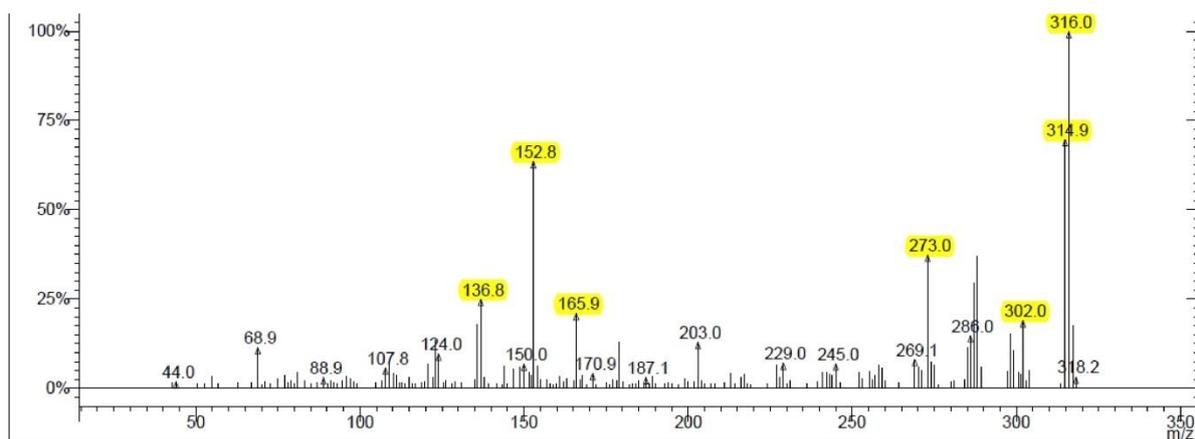


Figure S3. EI-MS spectrum of compound 6.

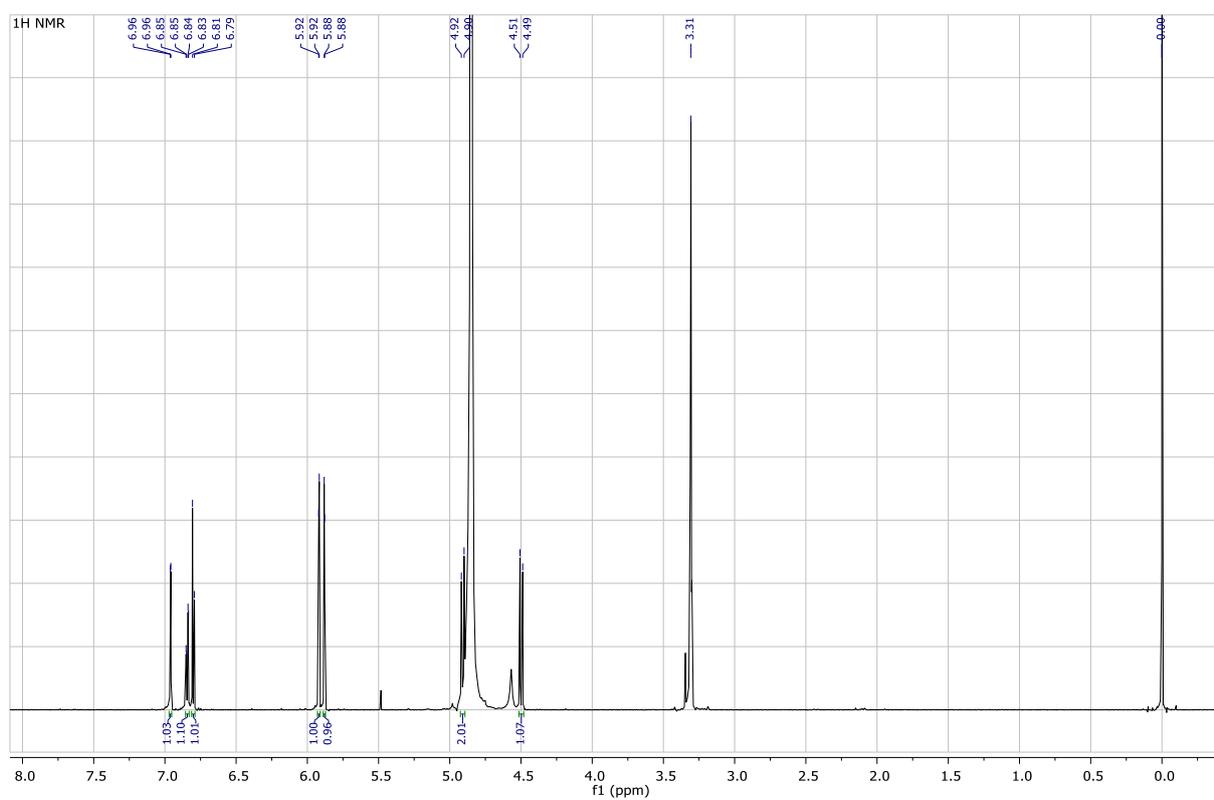


Figure S4. ¹H NMR spectrum (600 MHz, CD₃OD) of compound 7.

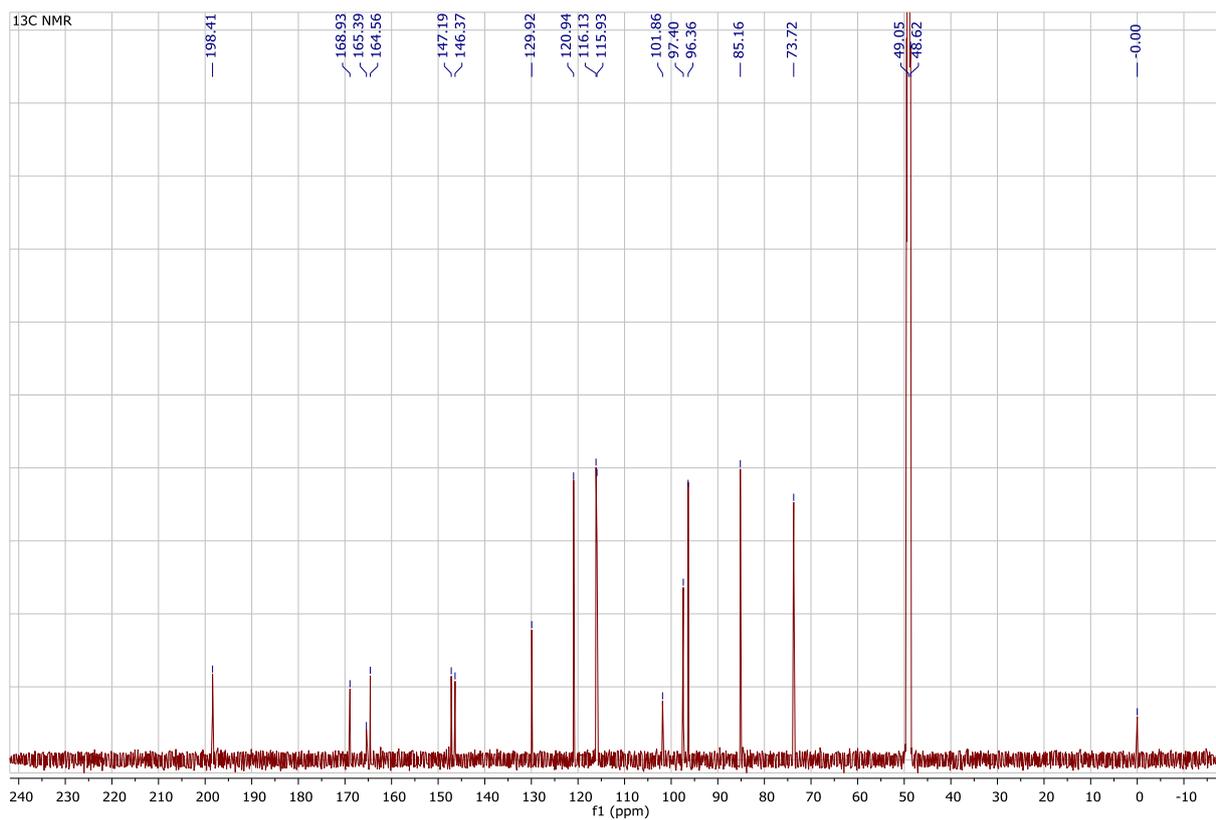


Figure S5. ¹³C NMR spectrum (150 MHz, CD₃OD) of compound 7.

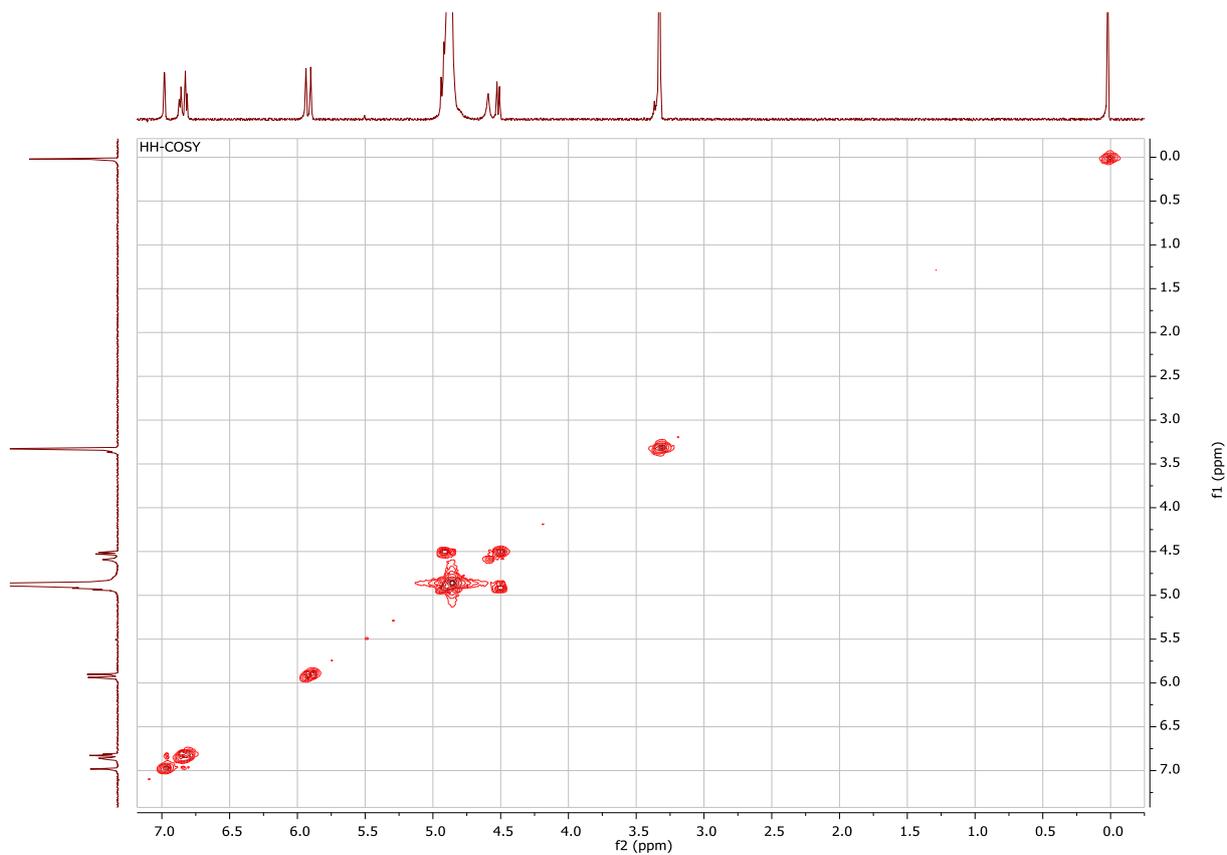


Figure S6. HH-COSY spectrum (600 MHz, CD₃OD) of compound 7.

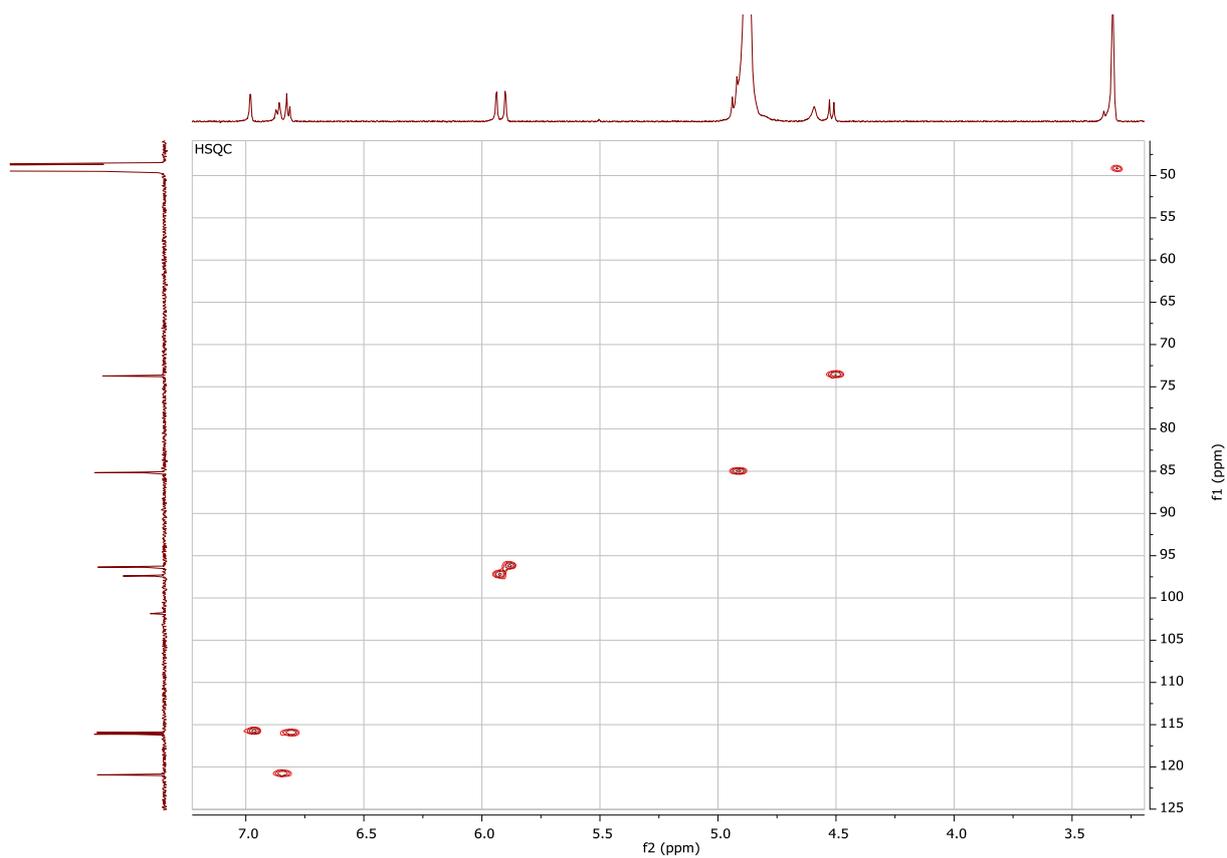


Figure S7. HSQC spectrum (600/150 MHz, CD₃OD) of compound **7**.

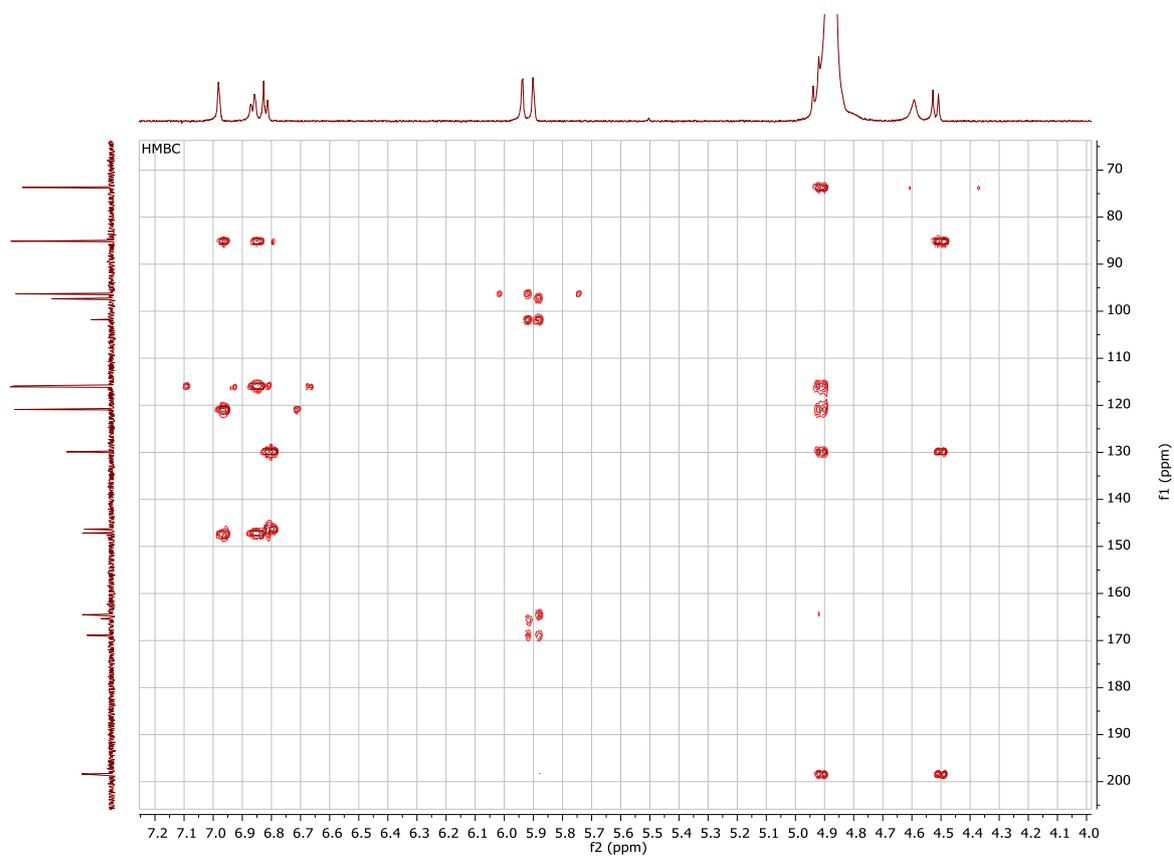


Figure S8. HMBC spectrum (600/150 MHz, CD₃OD) of compound **7**.

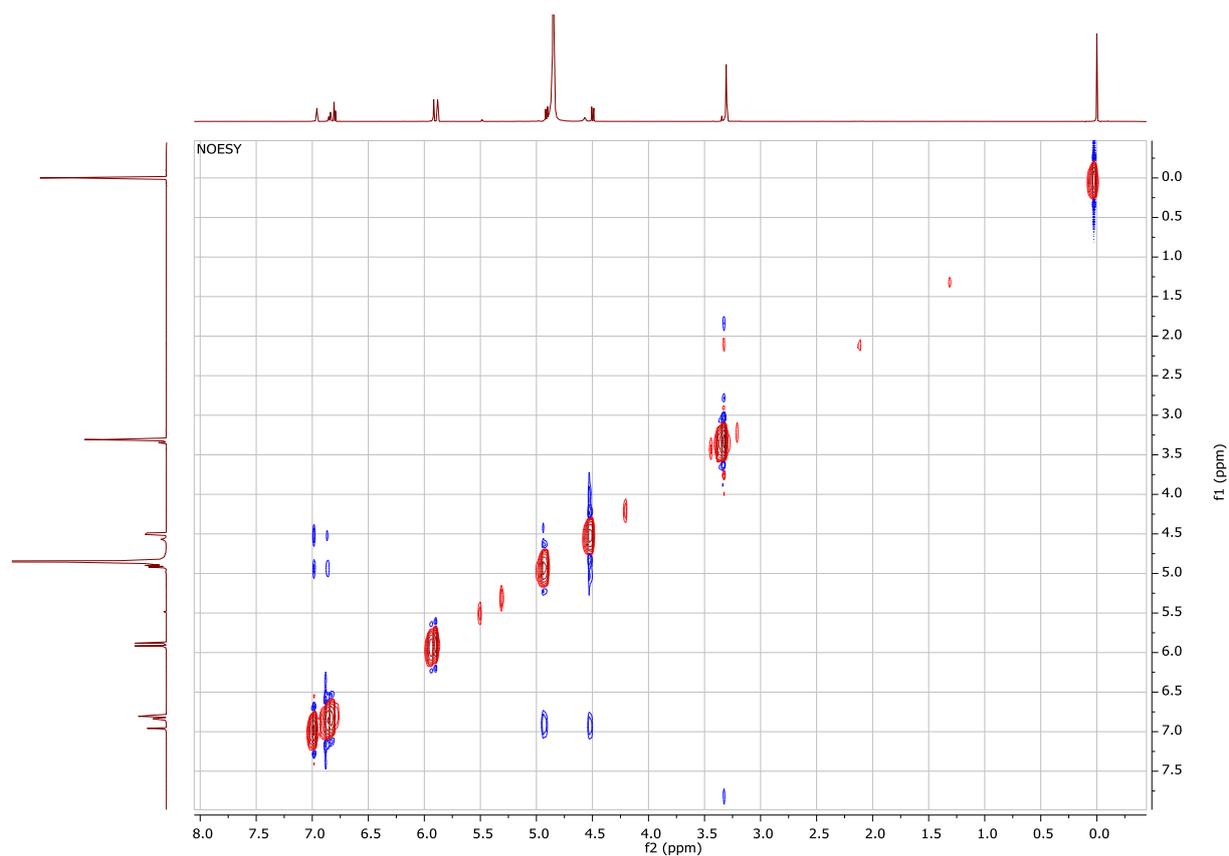


Figure S9. NOESY spectrum (600 MHz, CD₃OD) of compound **7**.

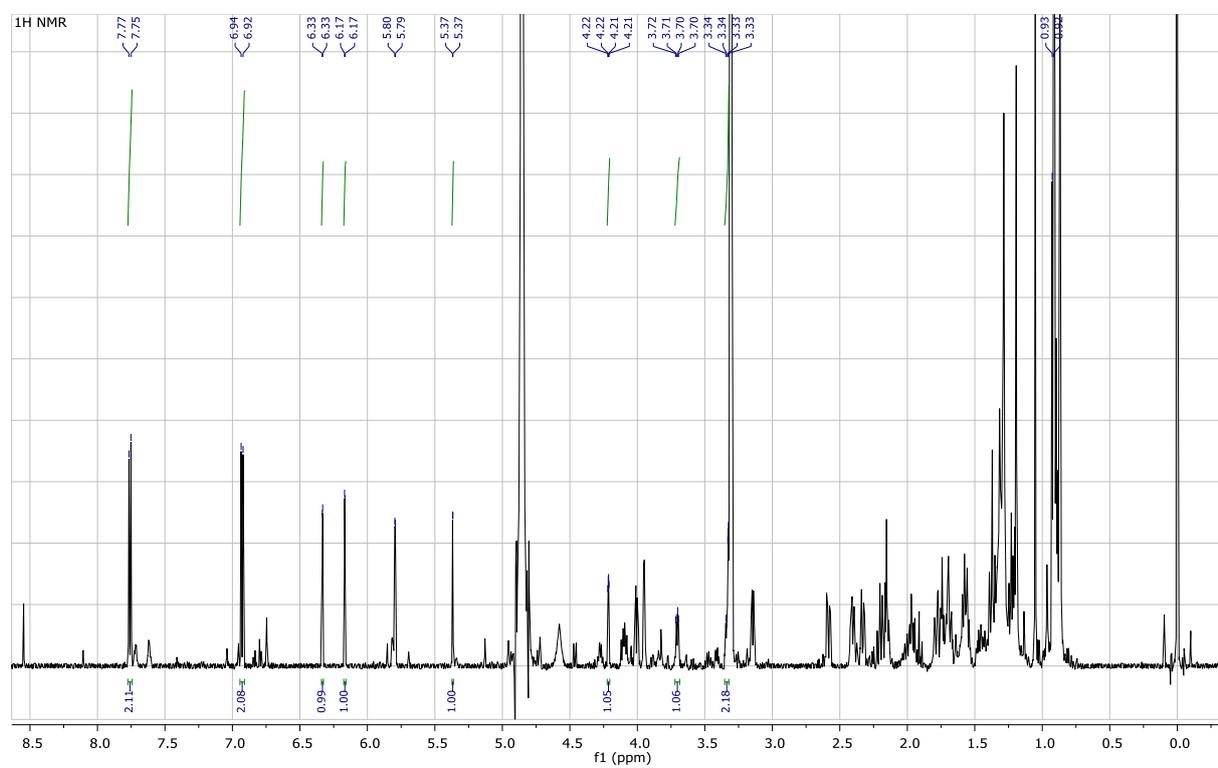


Figure S10. ¹H NMR spectrum (600 MHz, CD₃OD) of a mixture of compounds **8** and **9**. Only signals of compound **8** are labeled.

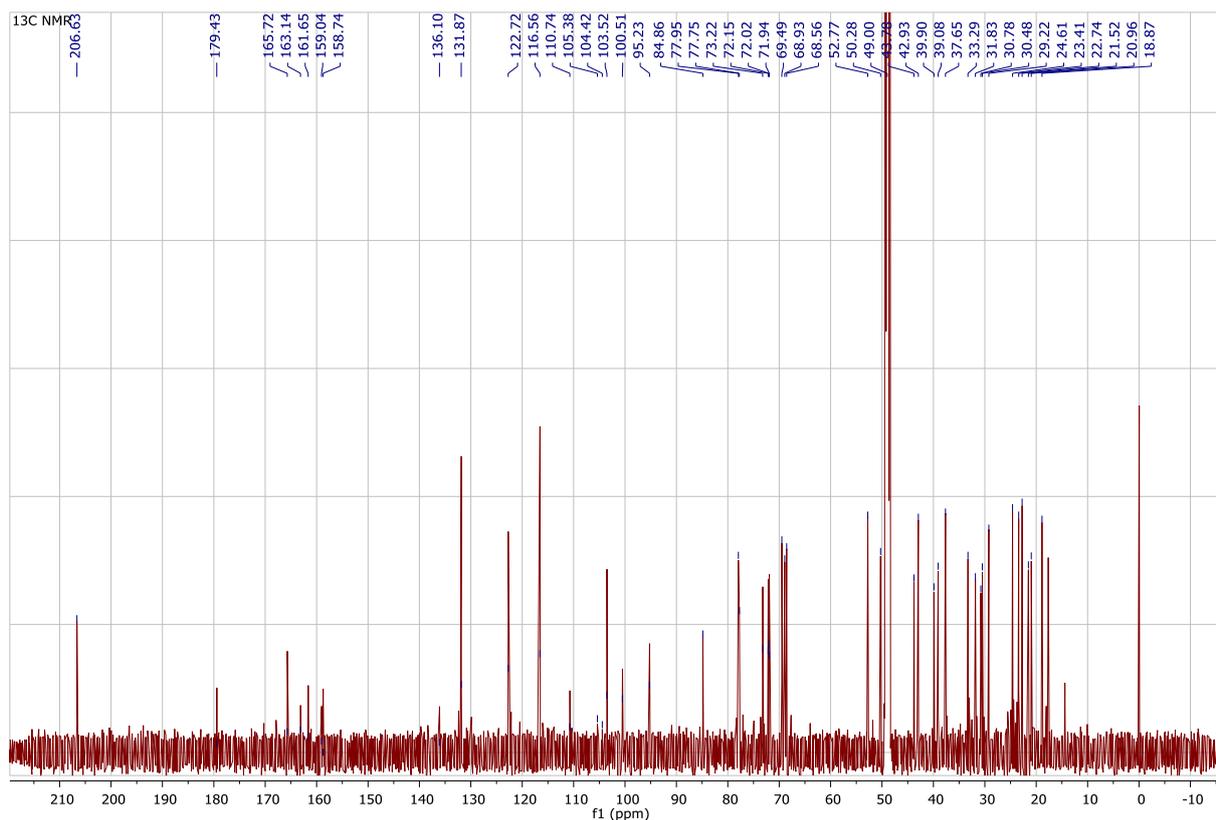


Figure S11. ^{13}C NMR spectrum (150 MHz, CD_3OD) of a mixture of compounds **8** and **9**.

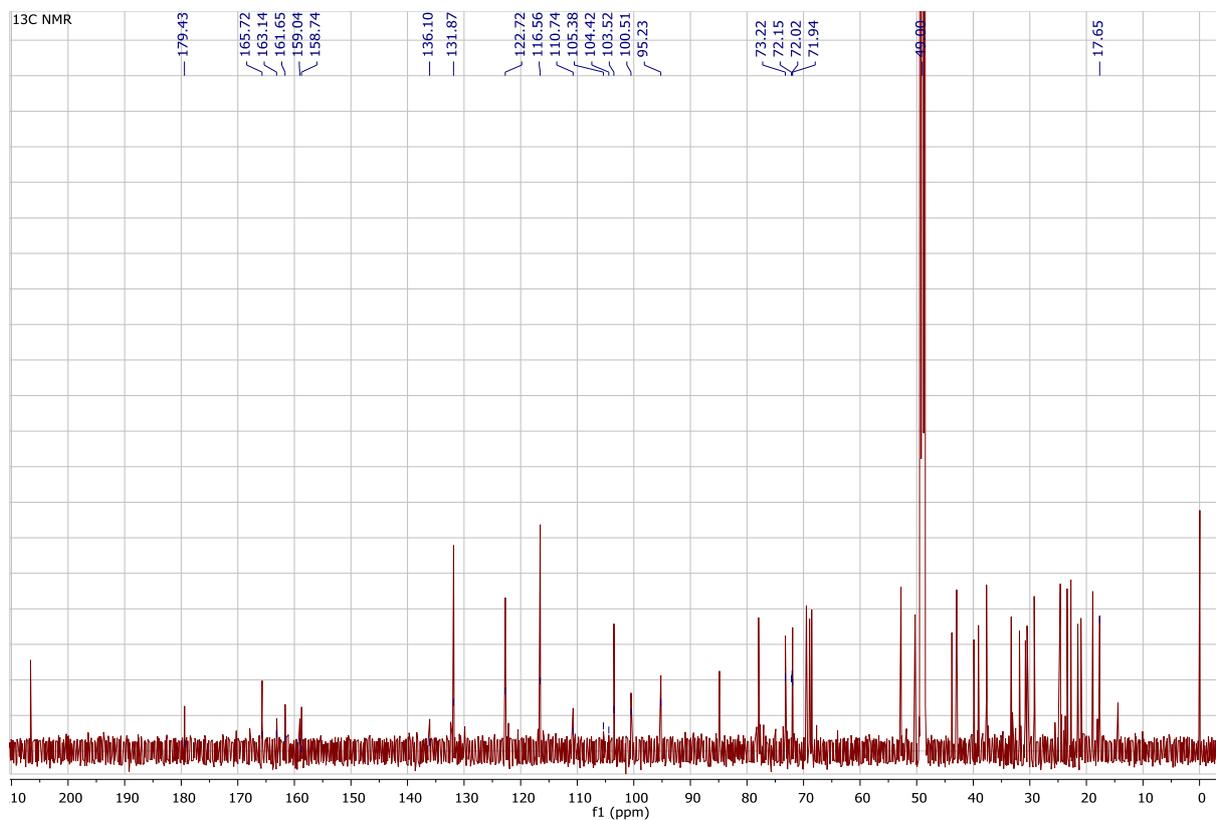


Figure S12. ^{13}C NMR spectrum (150 MHz, CD_3OD) of a mixture of compounds **8** and **9**. Only signals of compound **8** are labeled.

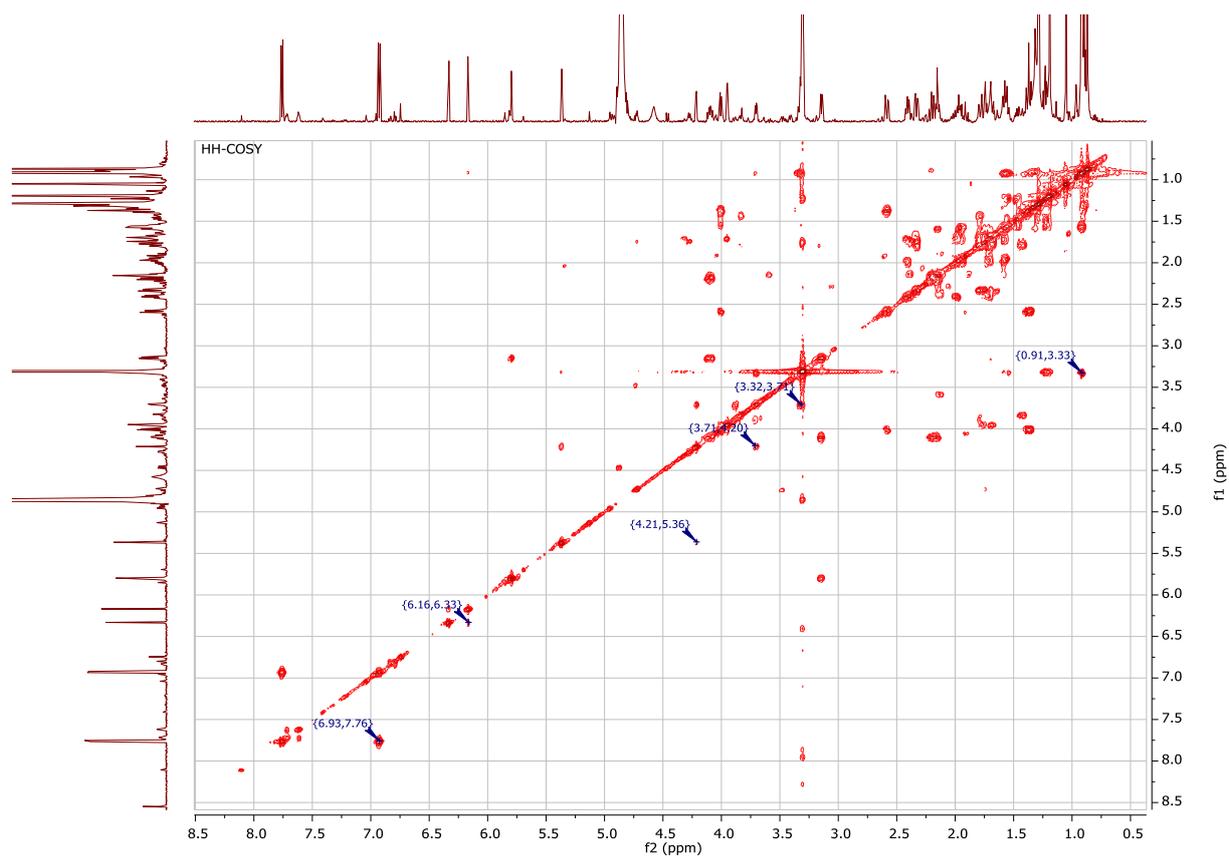


Figure S13. HH-COSY spectrum (600 MHz, CD₃OD) of a mixture of compounds **8** and **9**. Only signals of compound **8** are labeled.

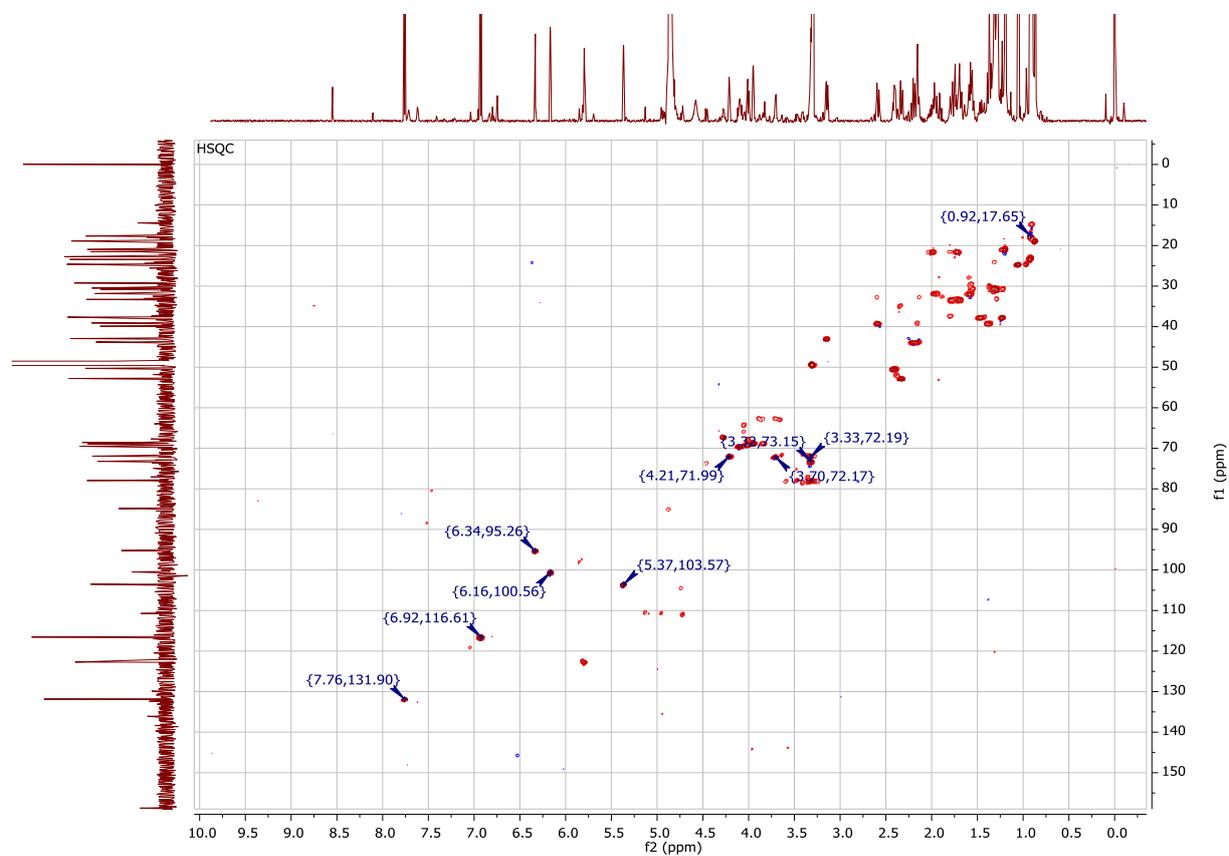


Figure S14. HSQC spectrum (600/150 MHz, CD₃OD) of a mixture of compounds **8** and **9**. Only signals of compound **8** are labeled.

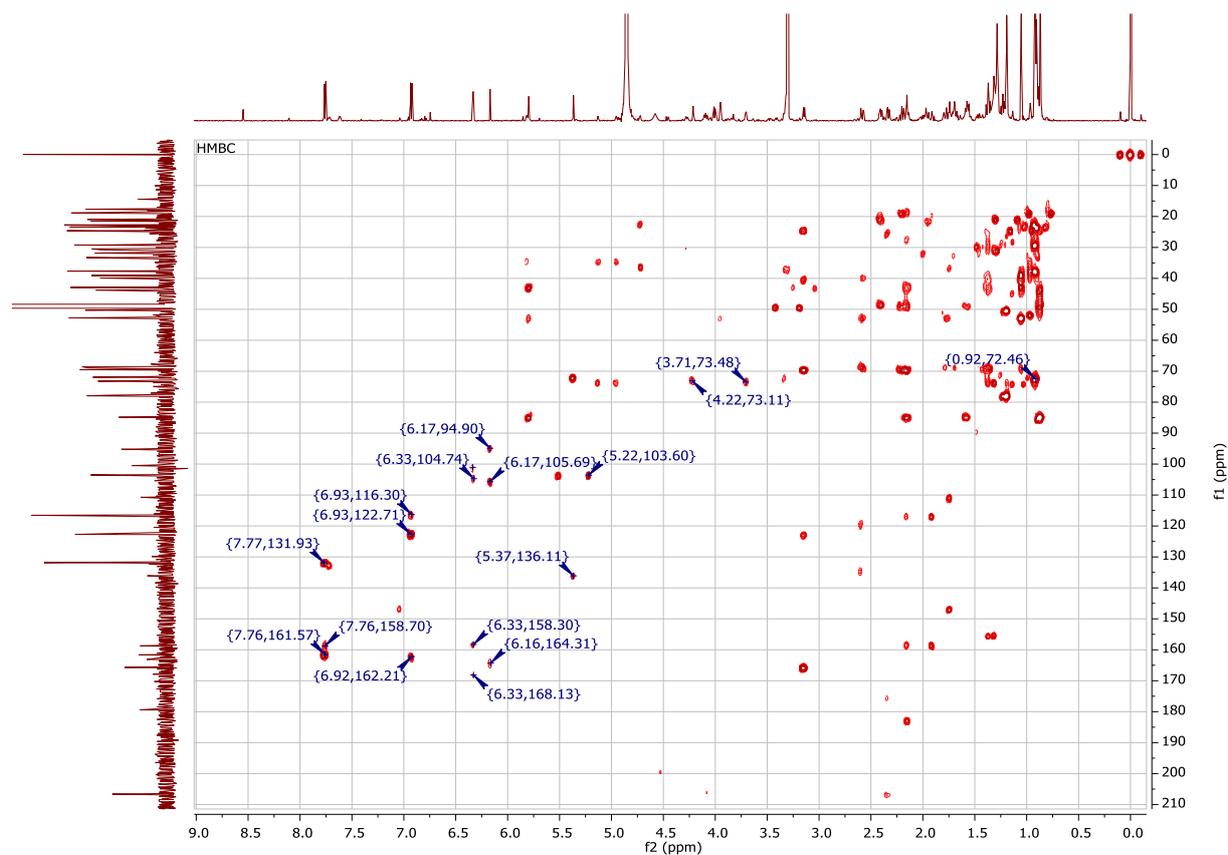


Figure S15. HMBC spectrum (600/150 MHz, CD₃OD) of a mixture of compounds **8** and **9**. Only signals of compound **8** are labeled.

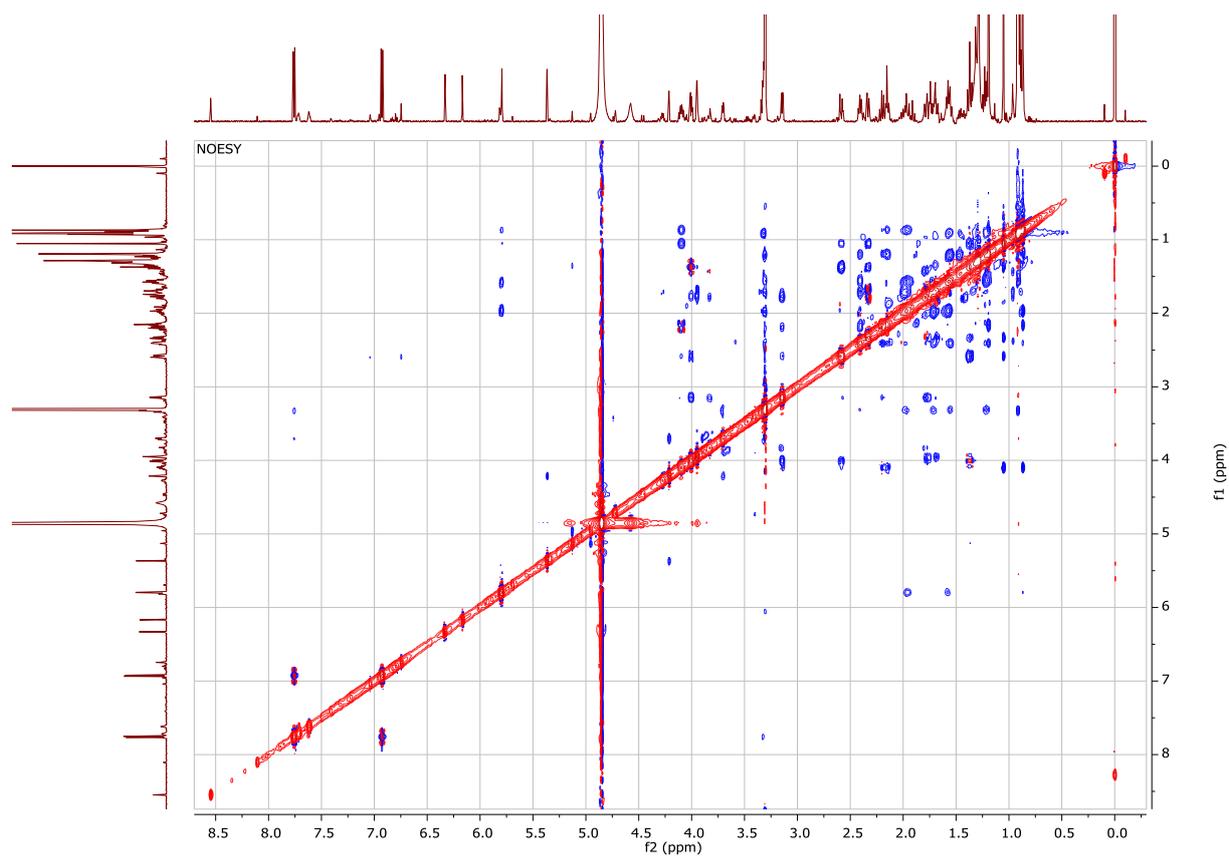


Figure S16. NOESY spectrum (600 MHz, CD₃OD) of a mixture of compounds **8** and **9**.

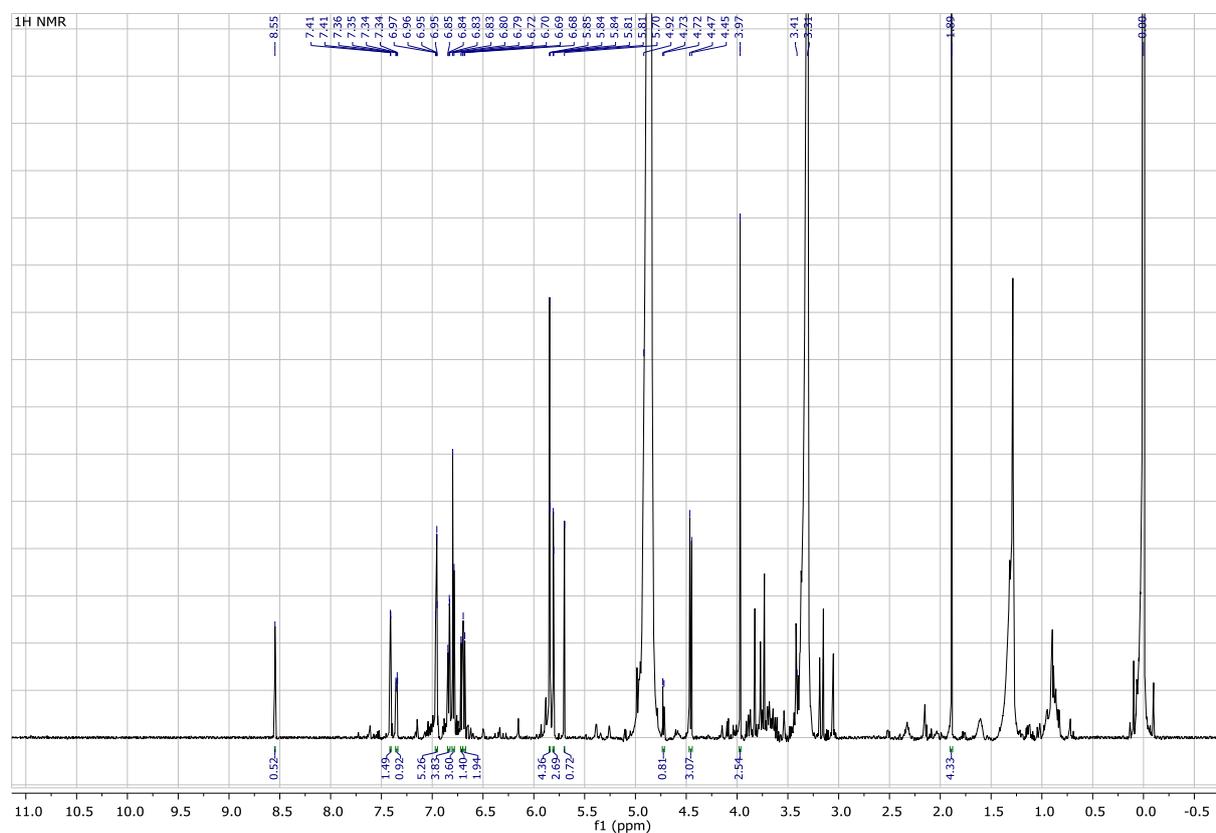


Figure S17. ¹H NMR spectrum (600 MHz, CD₃OD) of a mixture of compounds **7**, **10** and **11**.

Figure S20. ^1H NMR spectrum (600 MHz, CD_3OD) of a mixture of compounds **7**, **10** and **11**. Only signals of compound **7** are labeled.

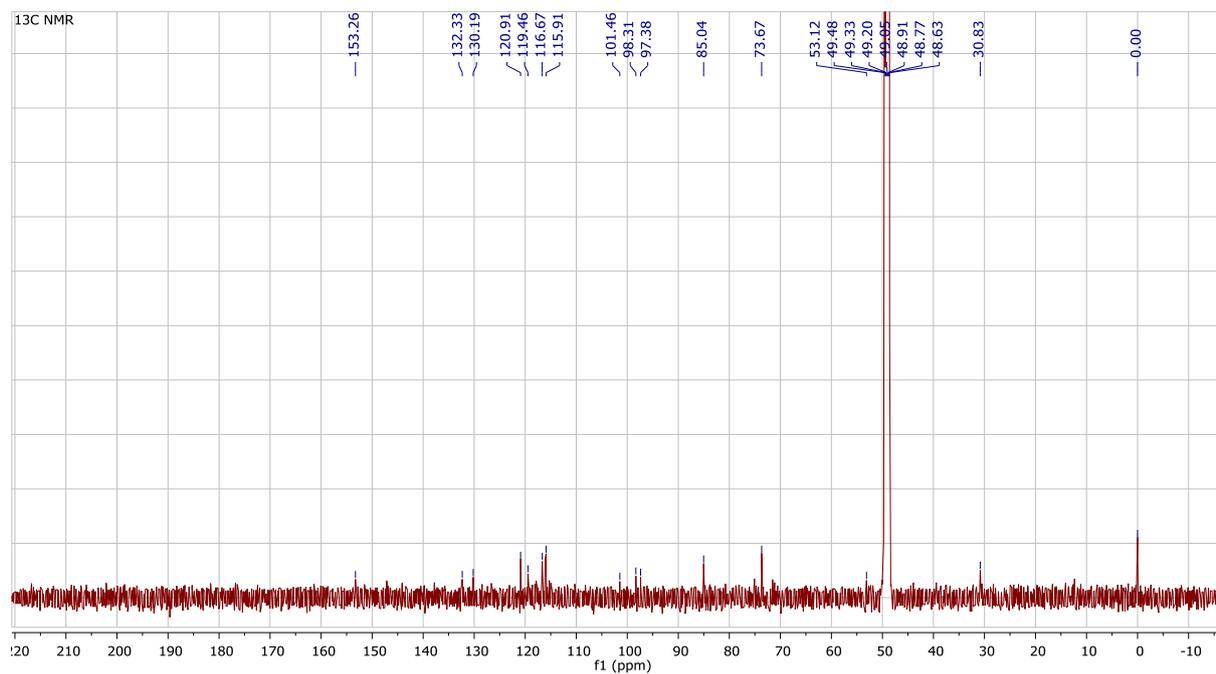


Figure S21. ^{13}C NMR spectrum (150 MHz, CD_3OD) of a mixture of compounds **7**, **10** and **11**.

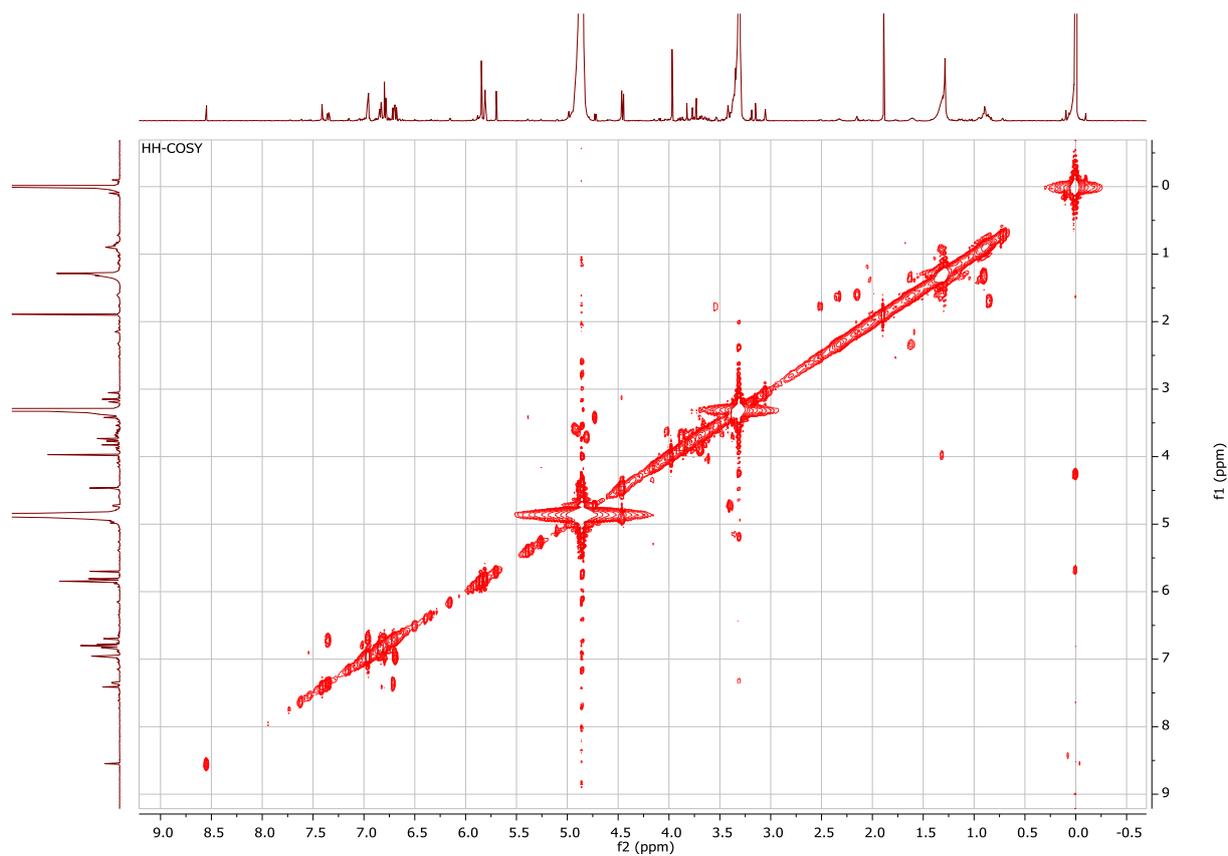


Figure S22. HH-COSY spectrum (600 MHz, CD_3OD) of a mixture of compounds **7**, **10** and **11**.

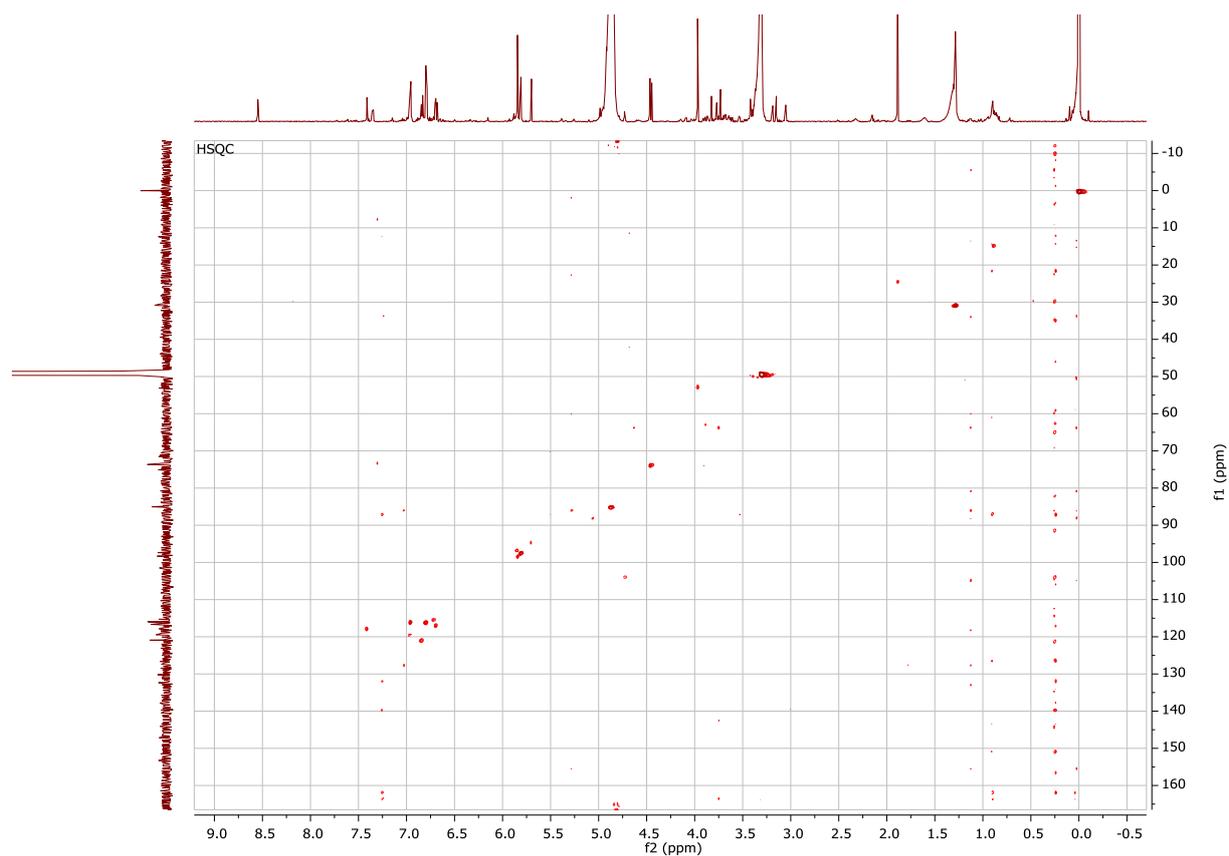


Figure S23. HSQC spectrum (600/150 MHz, CD₃OD) of a mixture of compounds **7**, **10** and **11**.

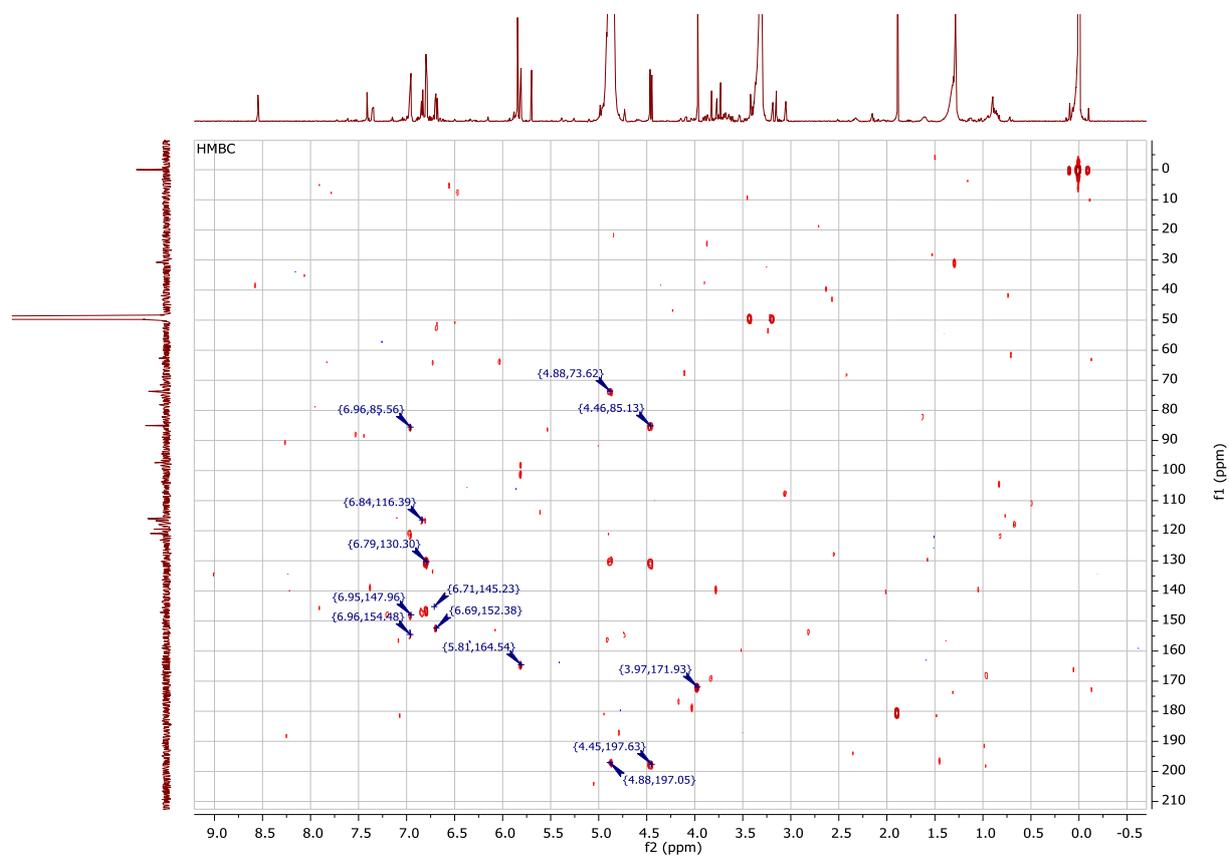


Figure S24. HMBC spectrum (600/150 MHz, CD₃OD) of a mixture of compounds **7**, **10** and **11**. The signals of compound **7** are labeled.

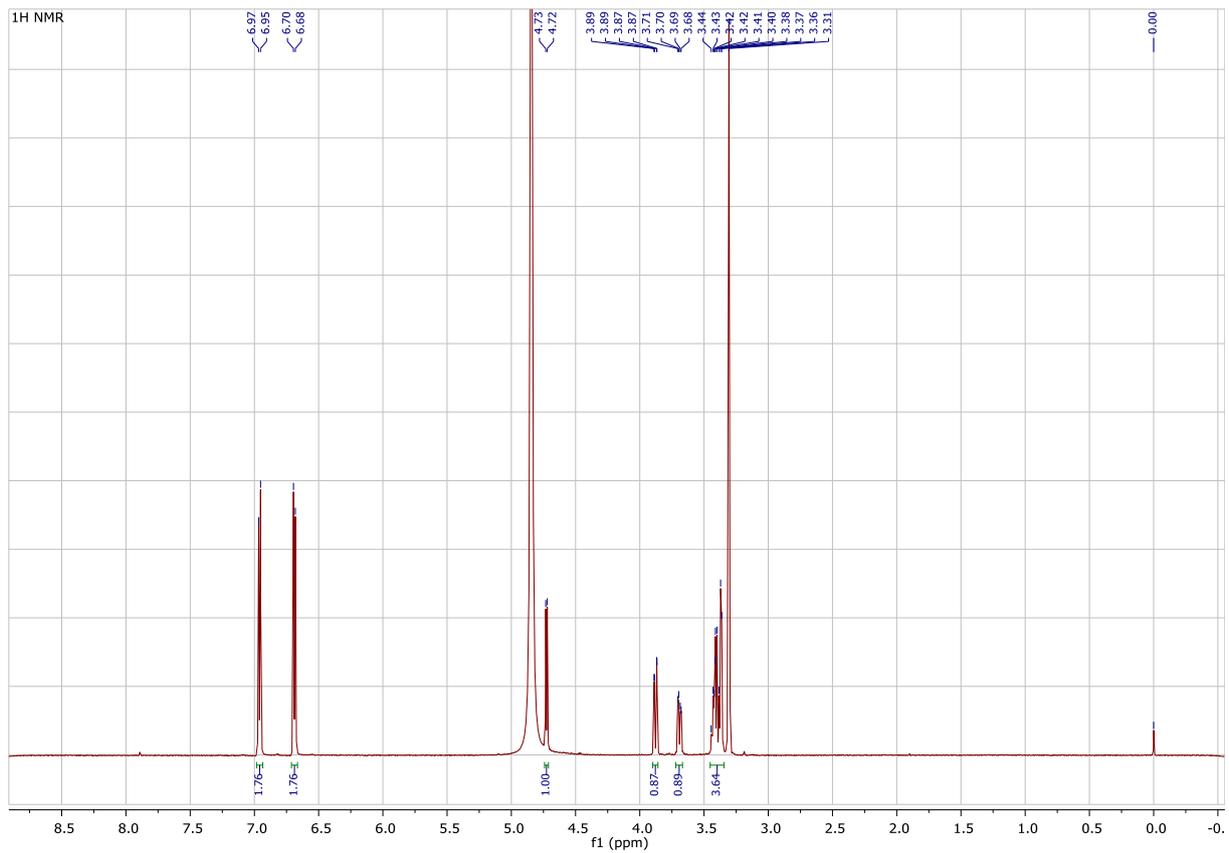


Figure S25. ¹H NMR spectrum (600 MHz, CD₃OD) of arbutin from *Serratula quinquefolia*.

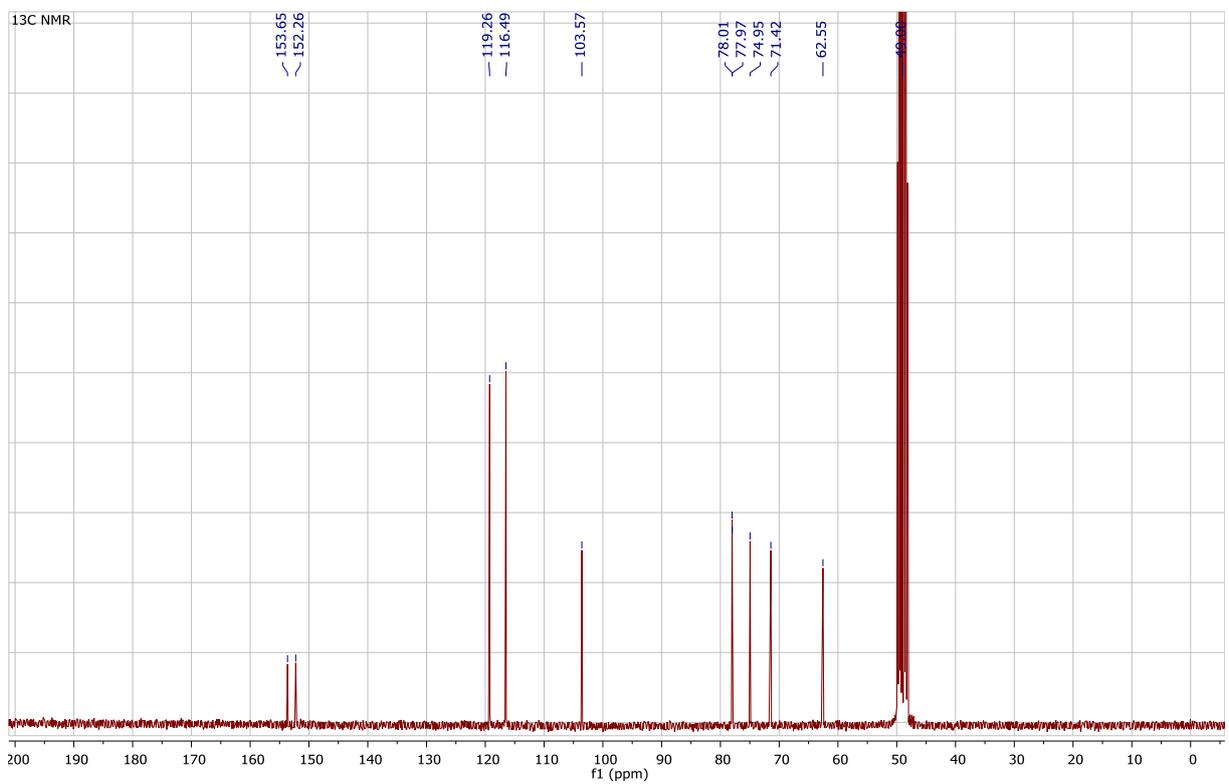


Figure S26. ¹³C NMR spectrum (150 MHz, CD₃OD) of arbutin from *Serratula quinquefolia*.

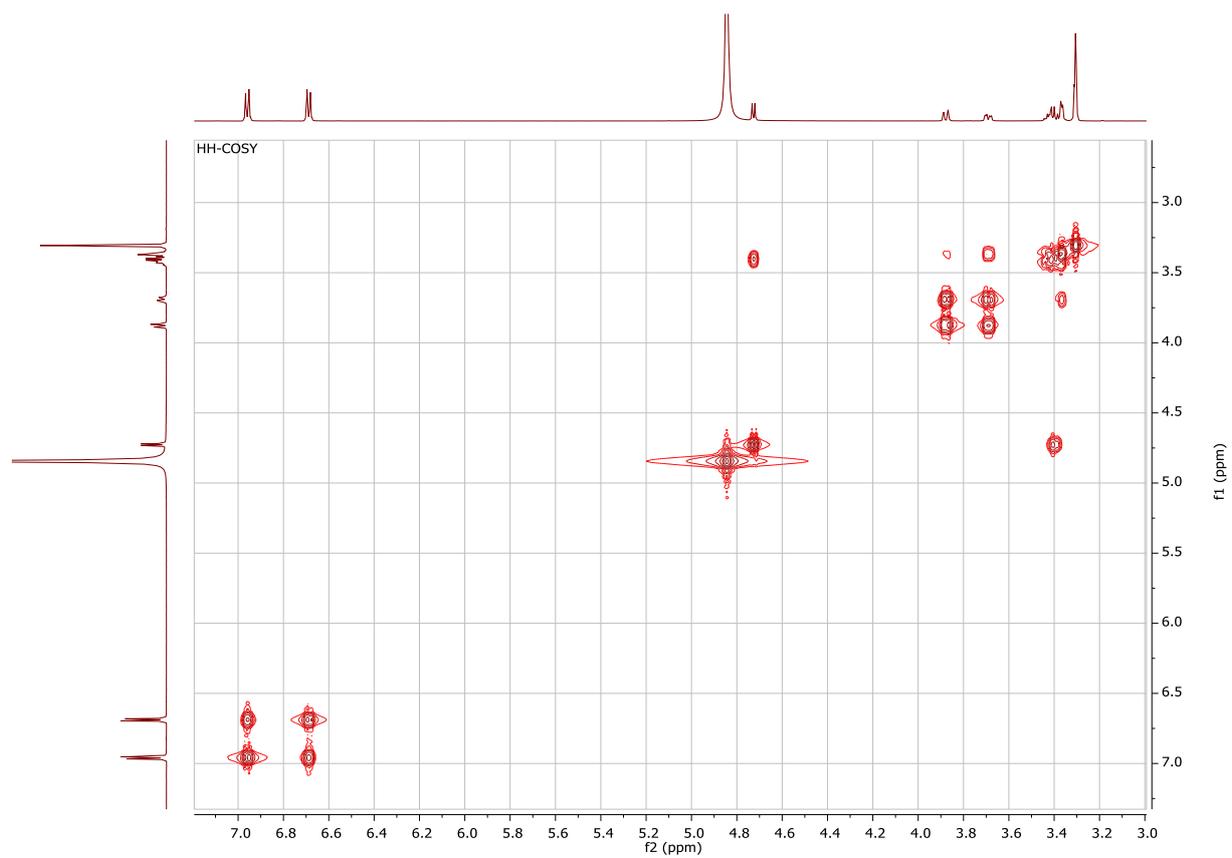


Figure S27. HH-COSY spectrum (600 MHz, CD₃OD) of arbutin from *Serratulaquinquefolia*.

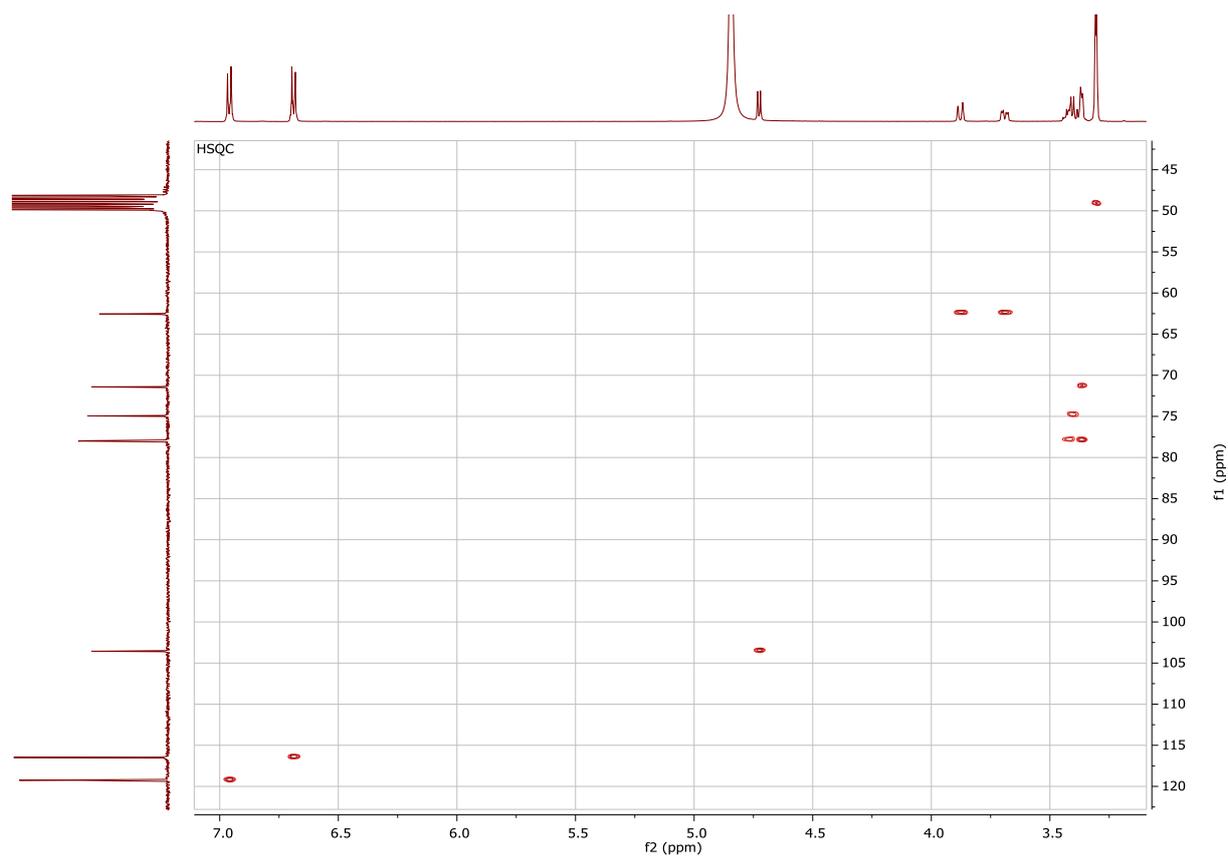


Figure S28. HSQC spectrum (600/150 MHz, CD₃OD) of arbutin from *Serratula quinquefolia*.

Table S1. NMR data (CD₃OD) of arbutin isolated from *Serratula quinquefolia*.

carbon	¹³ C δ _C	¹ H δ _H (Hz)
1		-
2	118.00	6.96 d (8.9)
3	115.20	6.69 d (8.9)
4		-
5	115.20	6.69 d (8.9)
6	118.00	6.96 d (8.9)
1'	102.26	4.73 d (7.3)
2'	73.57	3.40 dd (9.0, 7.3)
3'	76.63	3.43 t (9.0)
4'	70.09	3.53 m
5'	76.63	3.53 m
6'	61.18	3.88 dd (12.0, 1.3), 3.69 dd (12.0, 5.4)