

## Supplementary Materials

# New Napyradiomycin Analogues from *Streptomyces* sp. Strain CA-271078

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Received: 10 December 2019; Accepted: 25 December 2019; Published: date

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**Figure S38.** COSY spectrum of compound 5.

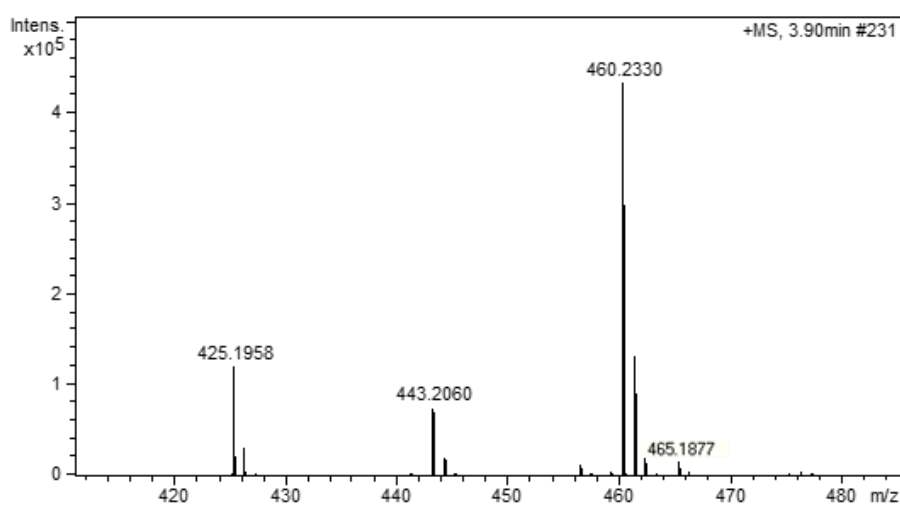
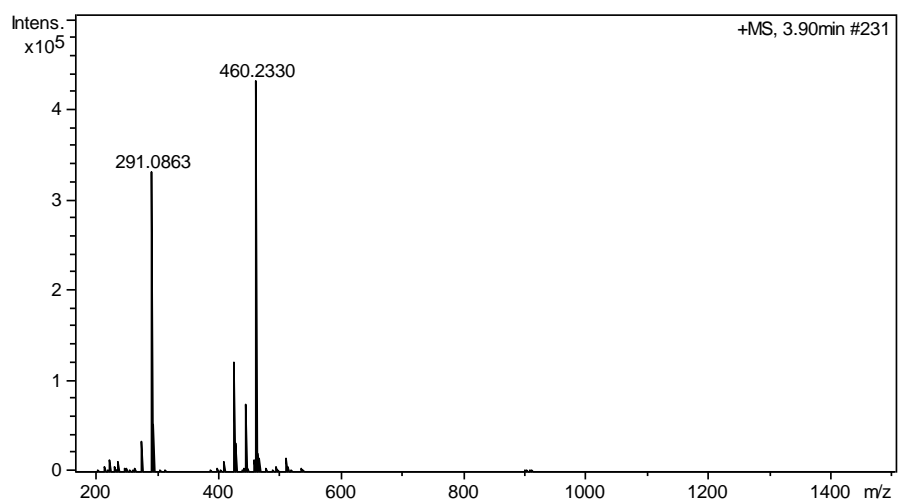
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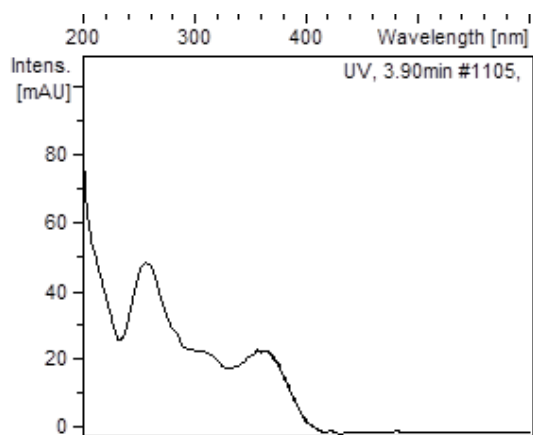
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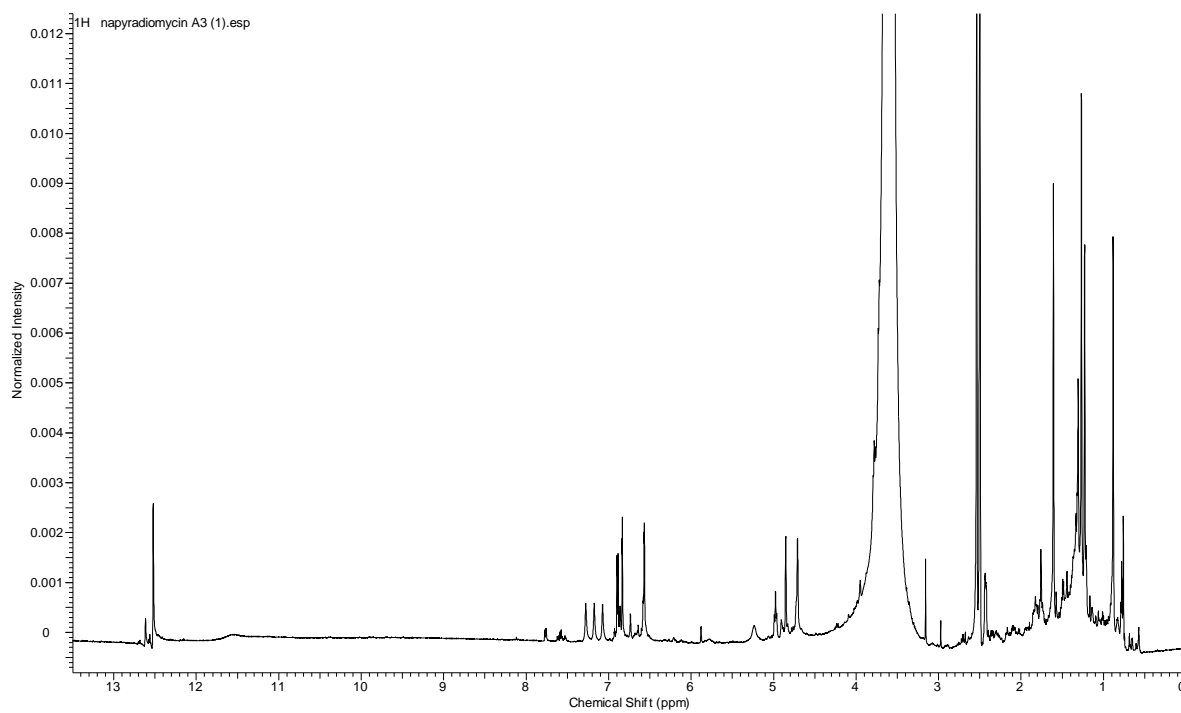


(A)

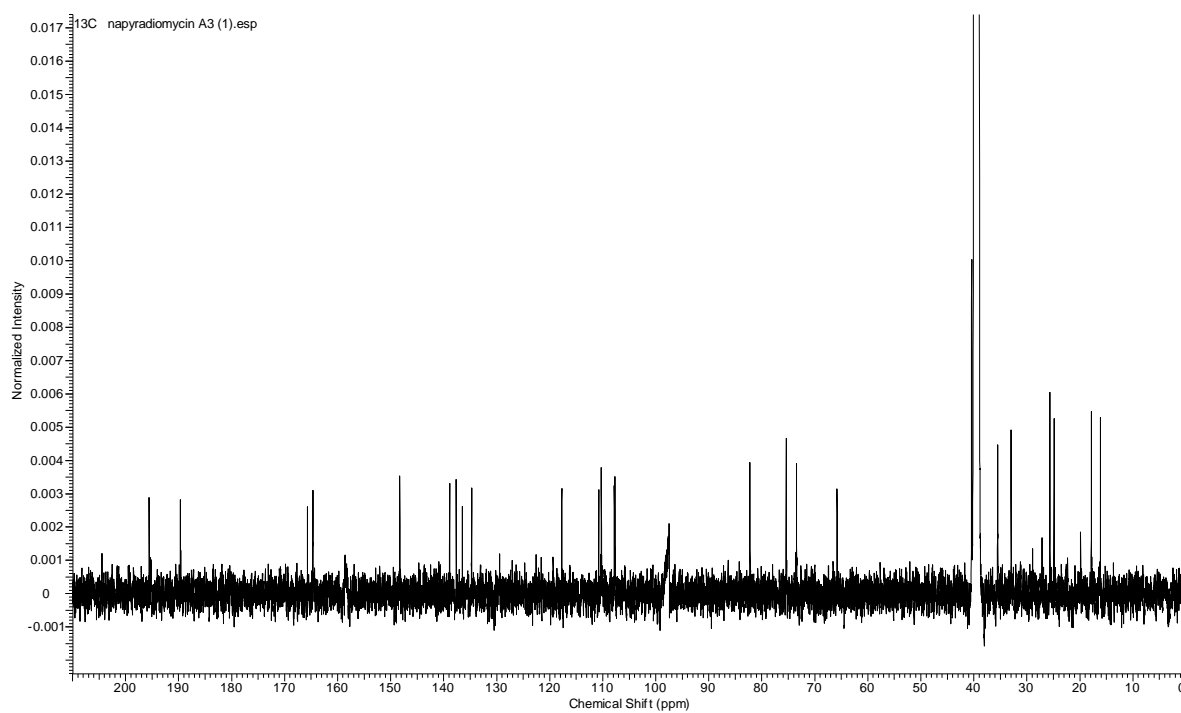


(B)

**Figure S1.** Electrospray-time of flight (ESI-TOF) (A) and UV (B) spectra of compound 1.



**Figure S2.** <sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 500 MHz) of compound 1.



**Figure S3.** <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 500 MHz) of compound 1.

COSY napradiomycin A3 (1).esp

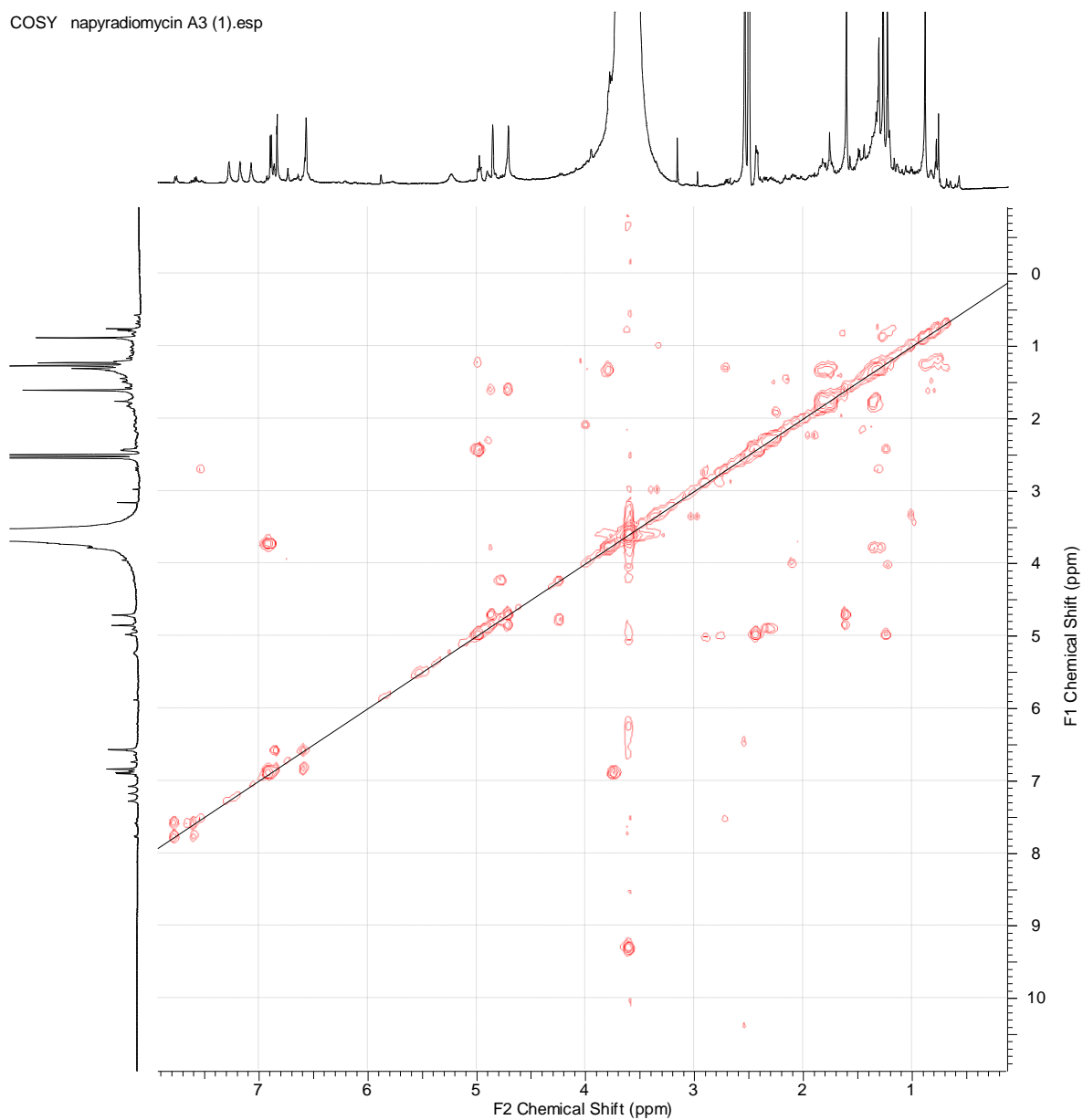
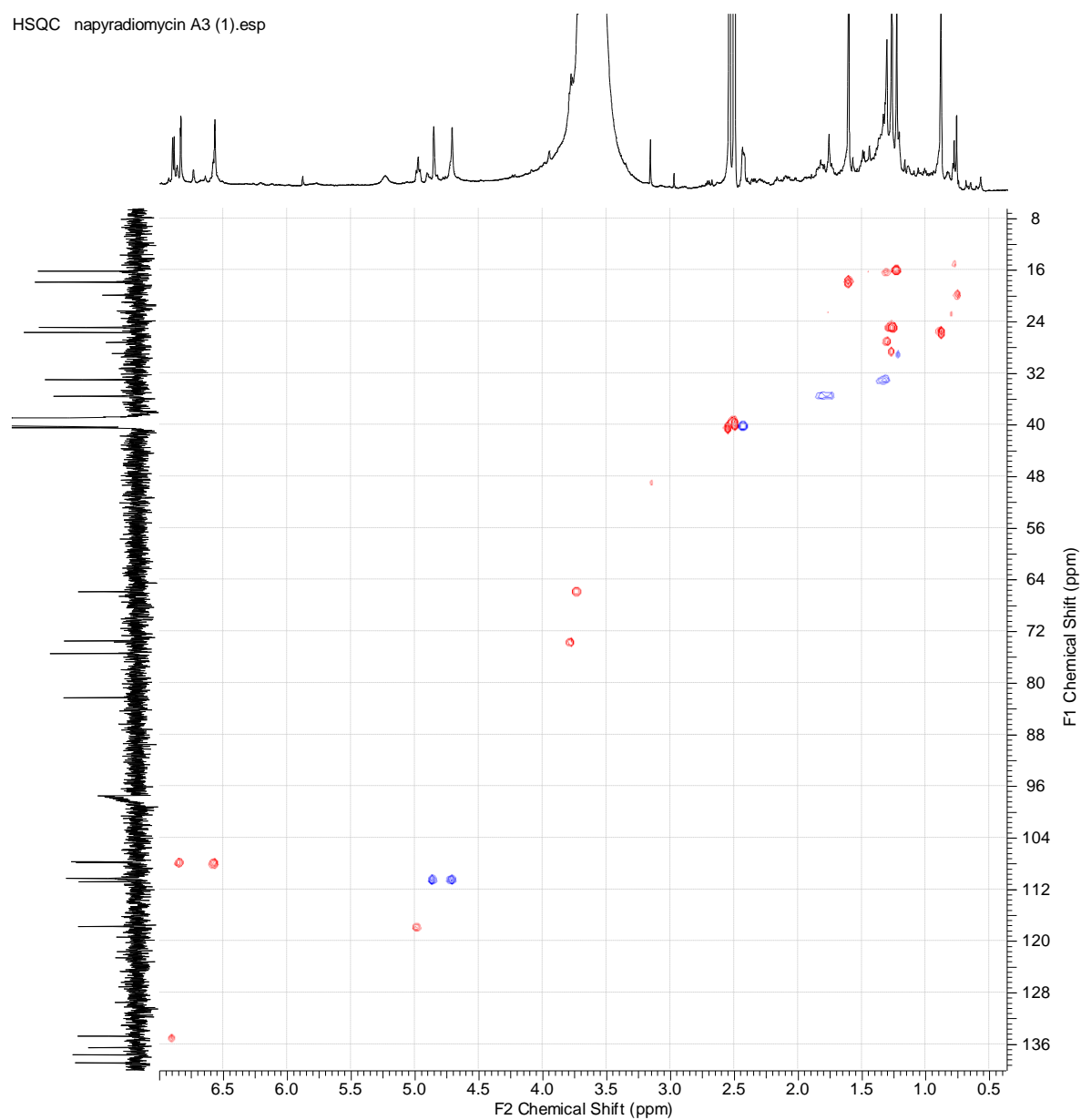


Figure S4. COSY of compound 1.

HSQC napyradiomycin A3 (1).esp

**Figure S5.** HSQC spectrum of compound 1.

HMBC napyradiomycin A3 (1).esp

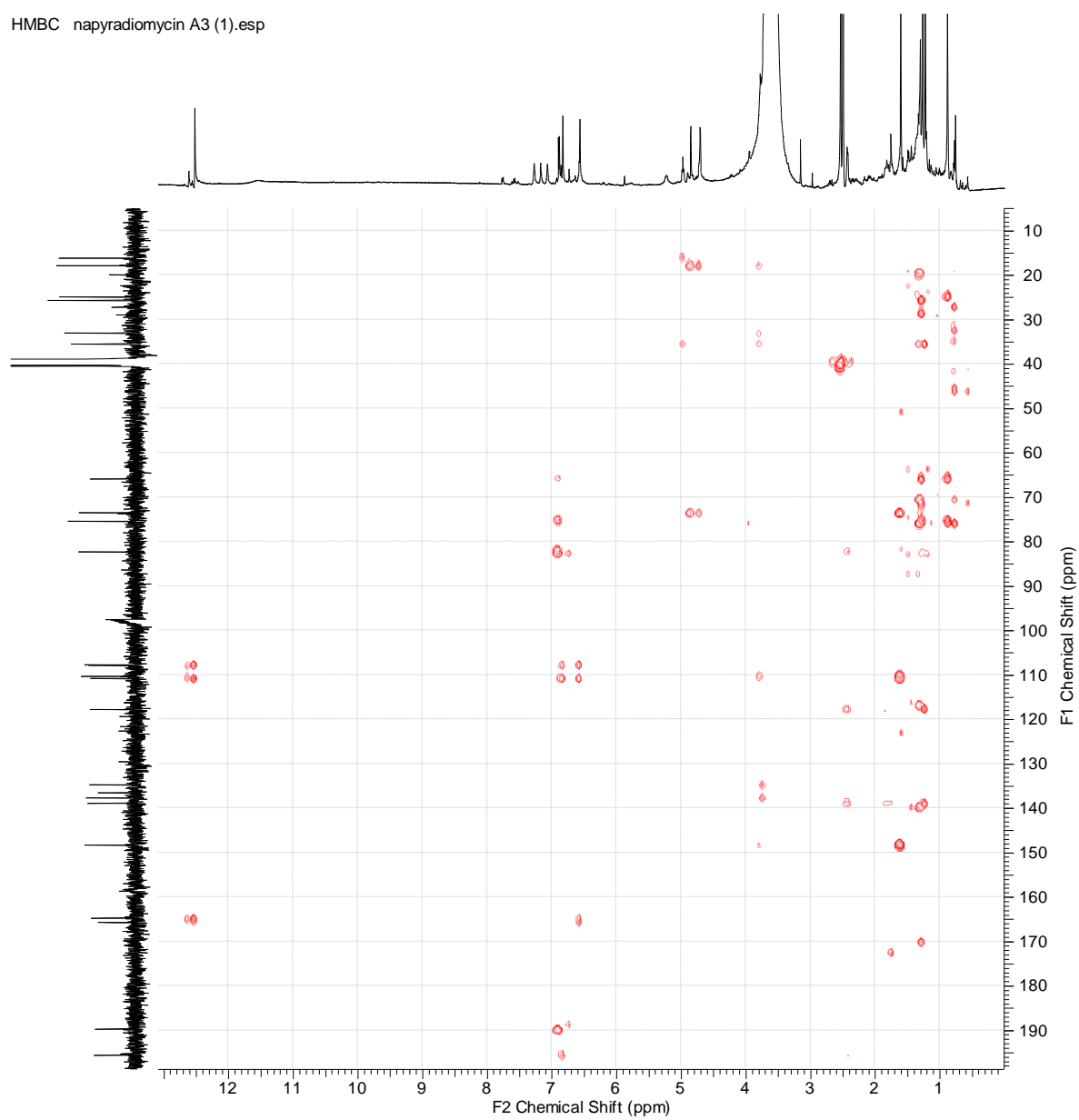


Figure S6. HMBC of compound 1.

ROESY napyradiomycin A3 (1).esp

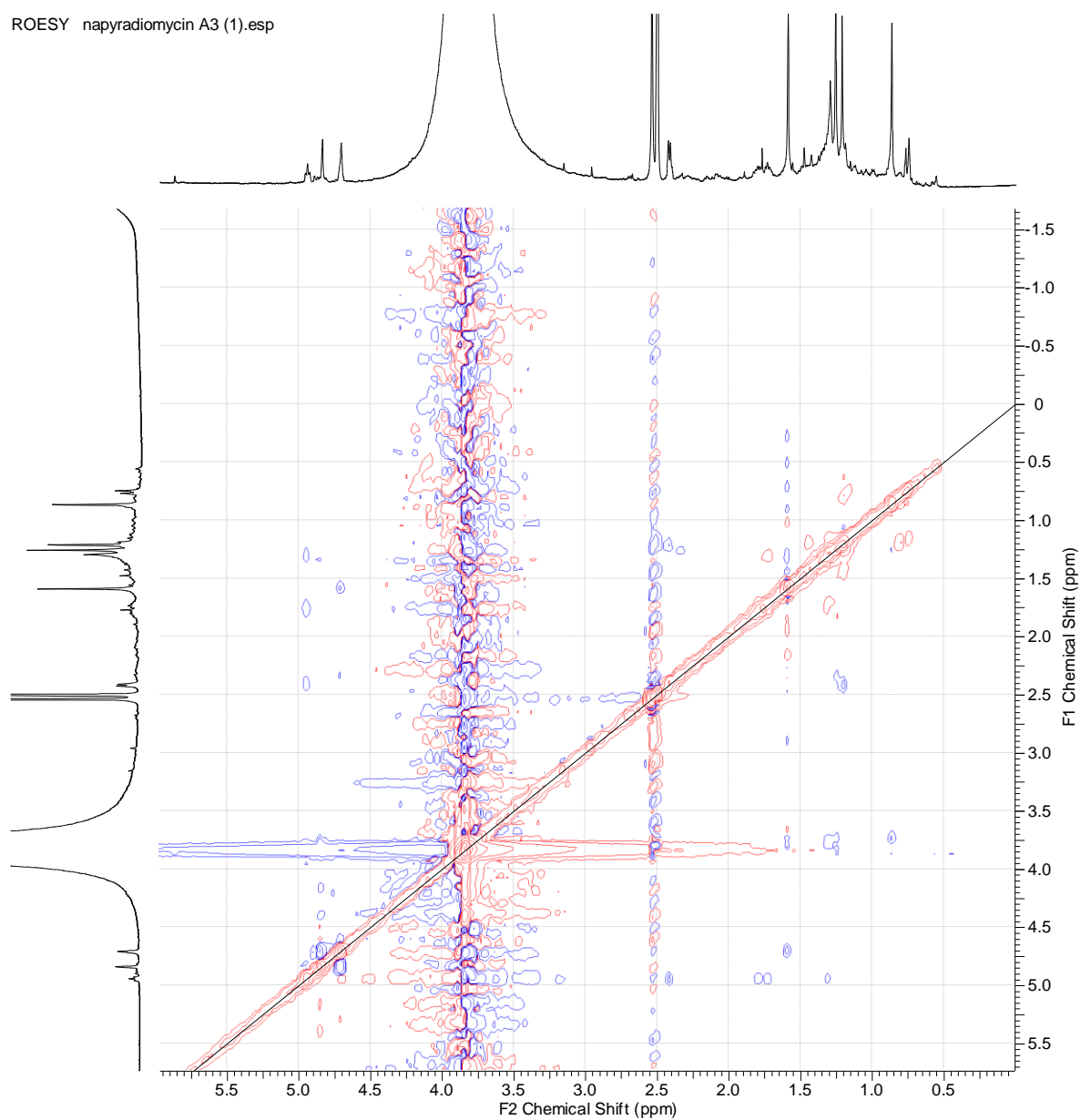
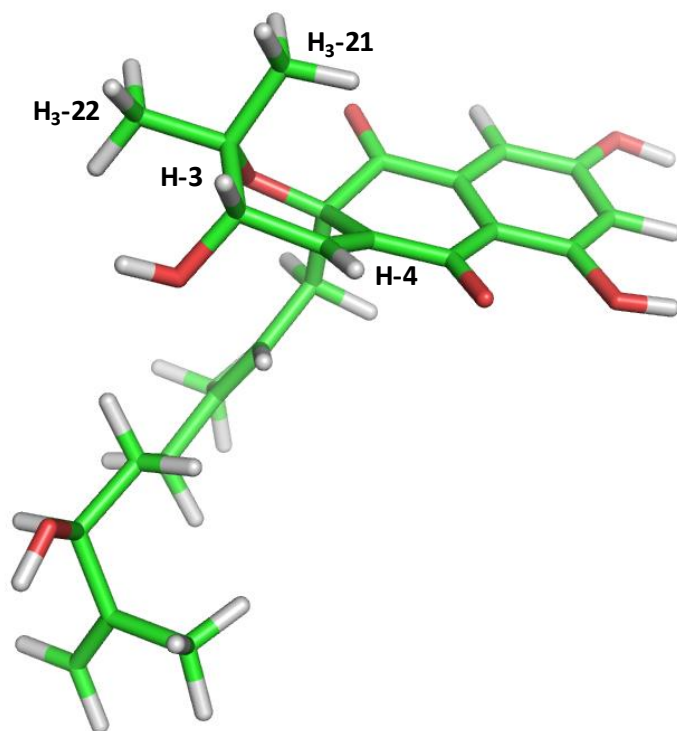
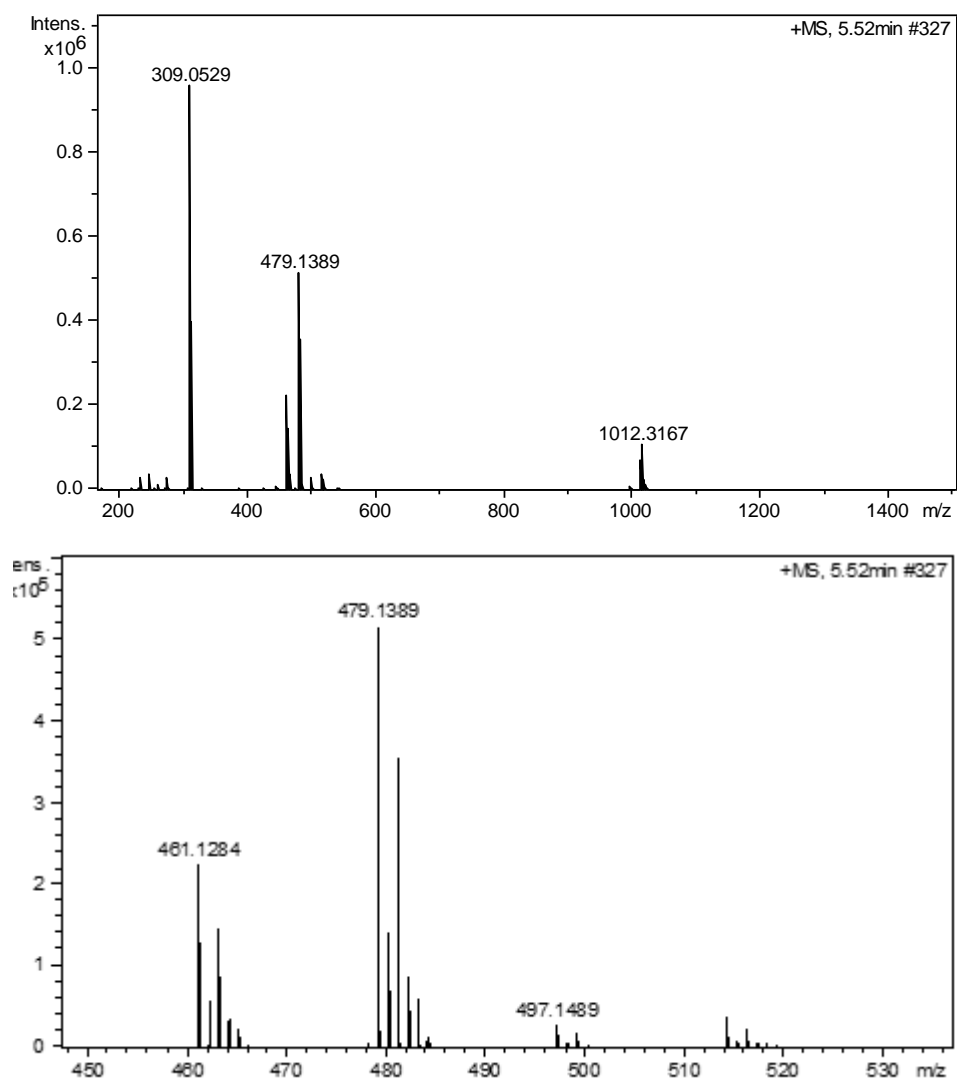


Figure S7. ROESY of compound 1

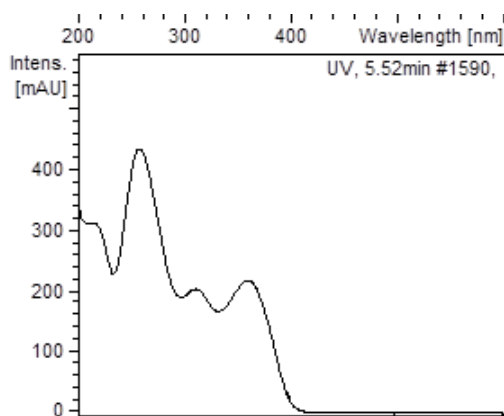




**Figure S8.** Energy minimized molecular model of compound 1.

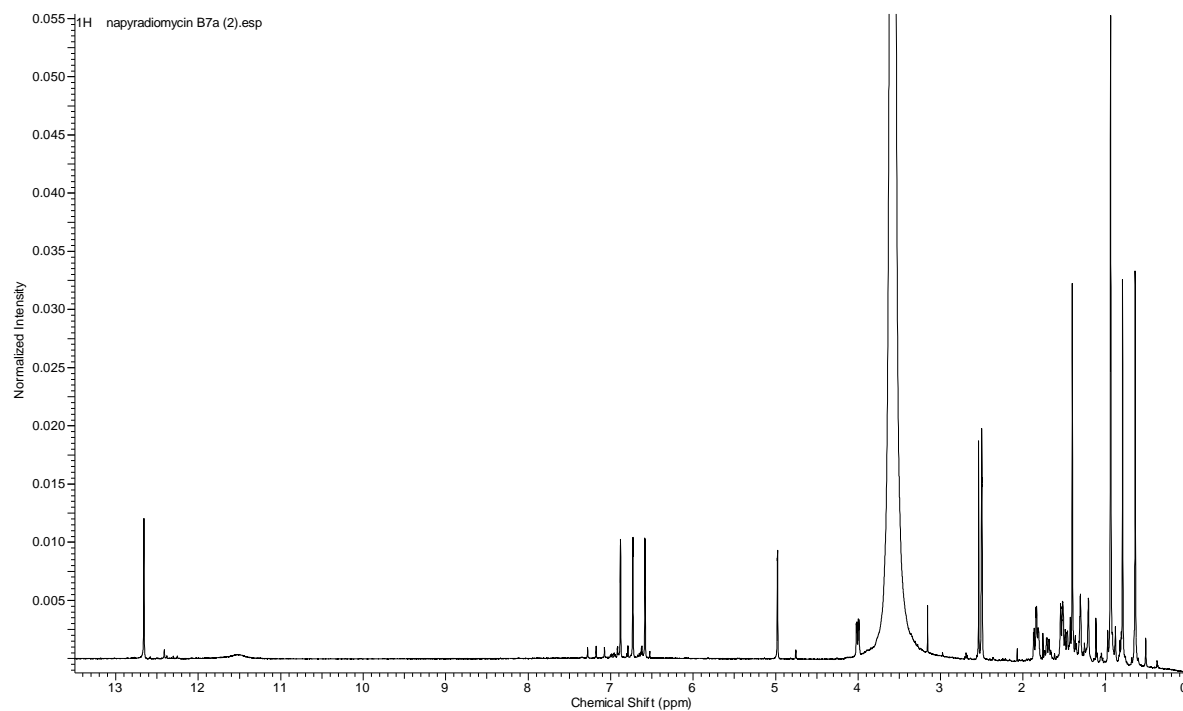


(A)

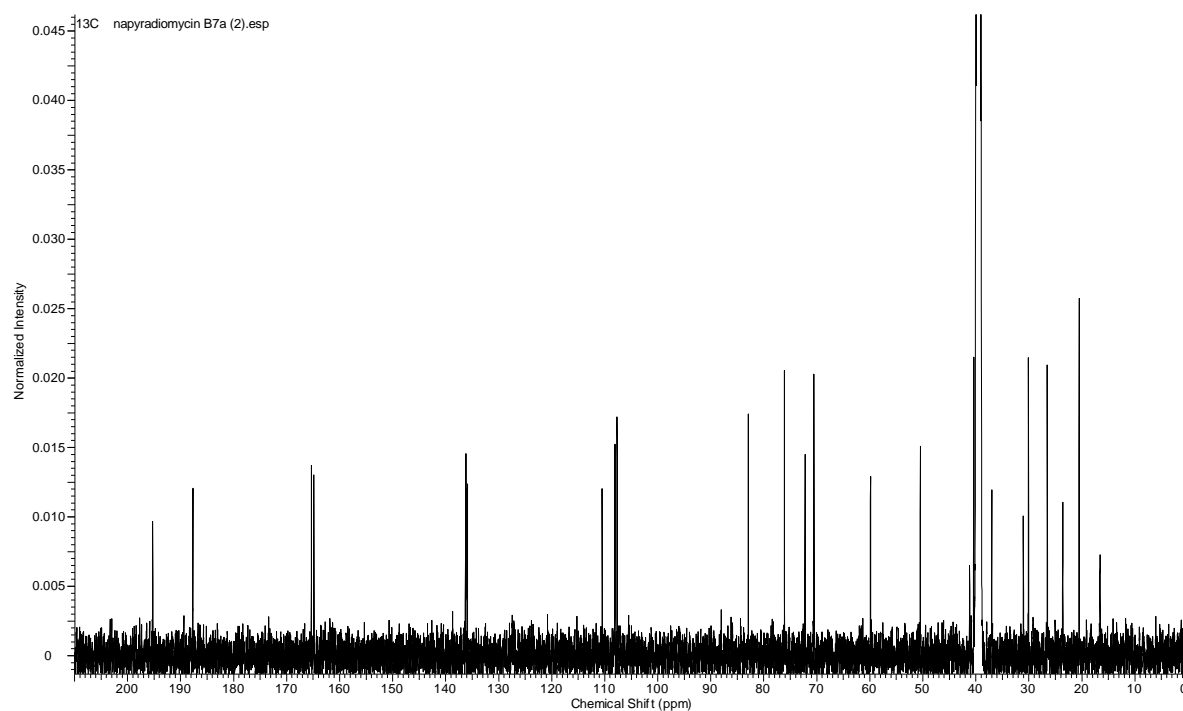


(B)

**Figure S9.** Electrospray-time of flight (ESI-TOF) (A) and UV (B) spectra of compound 2.



**Figure S10.** <sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 500 MHz) of compound **2**.



**Figure S11.** <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 500 MHz) of compound **2**.



HSQC napyradiomycin B7a (2).esp

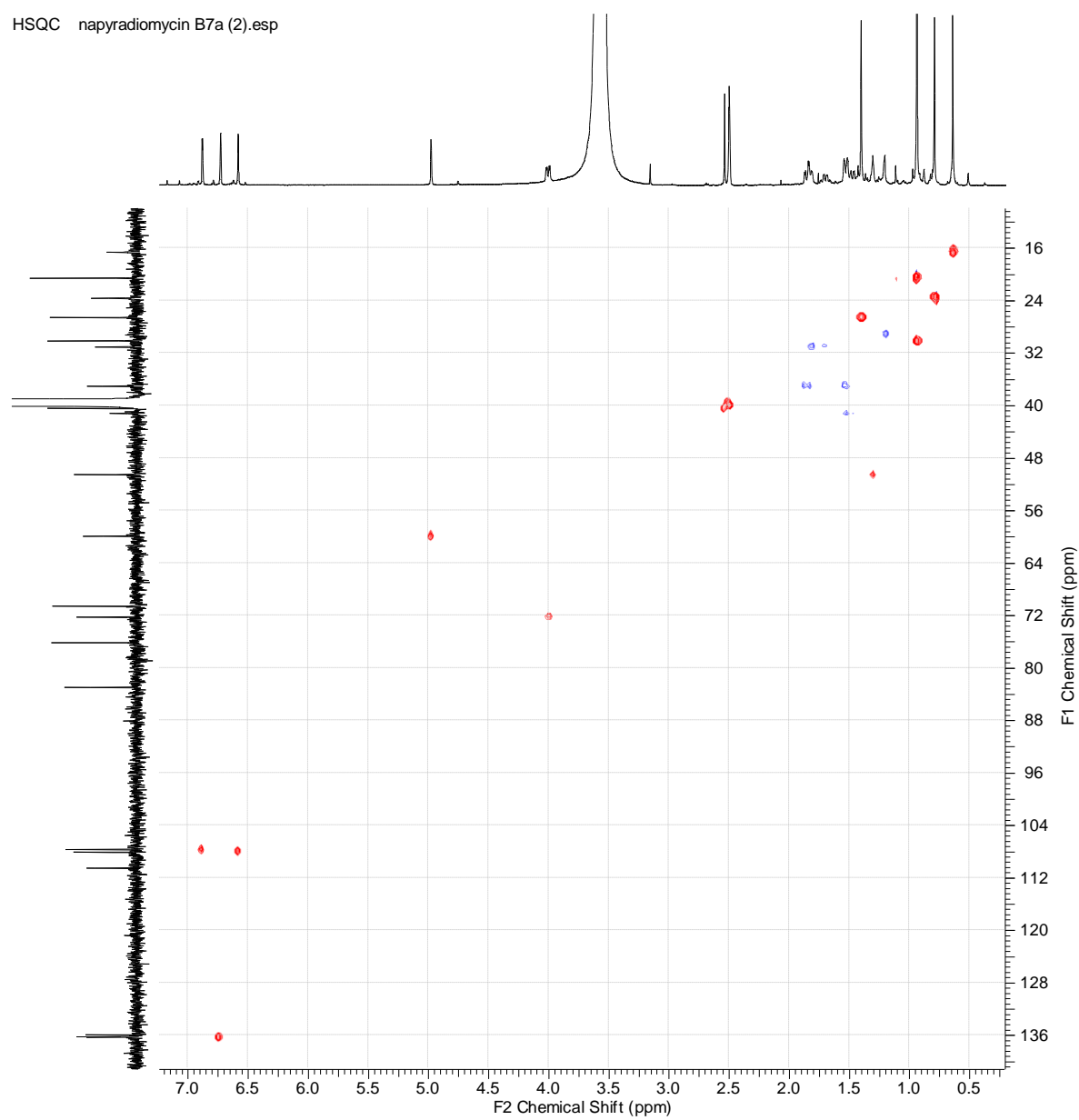


Figure S13. HSQC spectrum of compound 2.

HMBC napyradiomycin B7a (2).esp

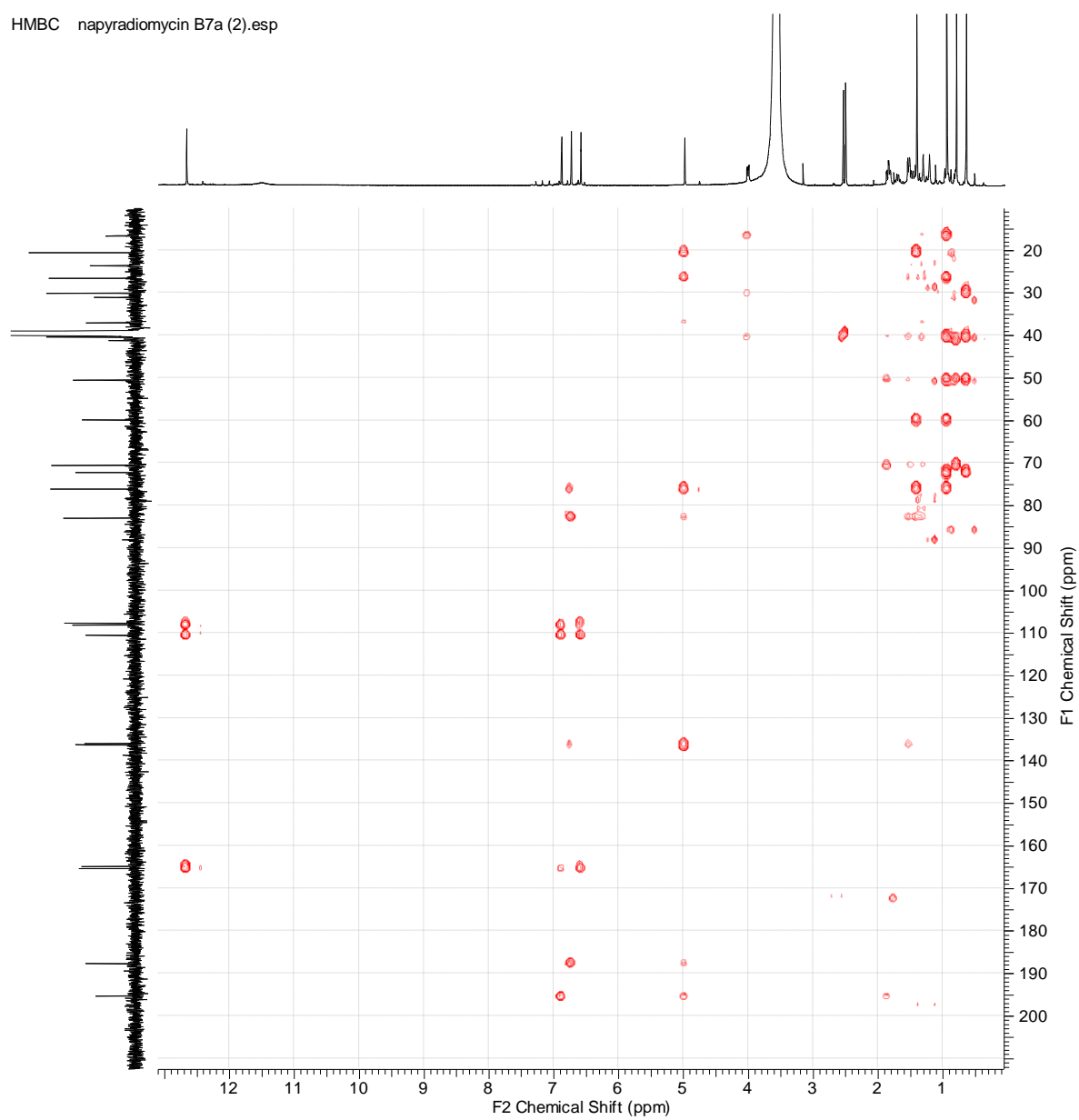


Figure S14. HMBC of compound 2.

NOESY napyradiomycin B7a (2).esp

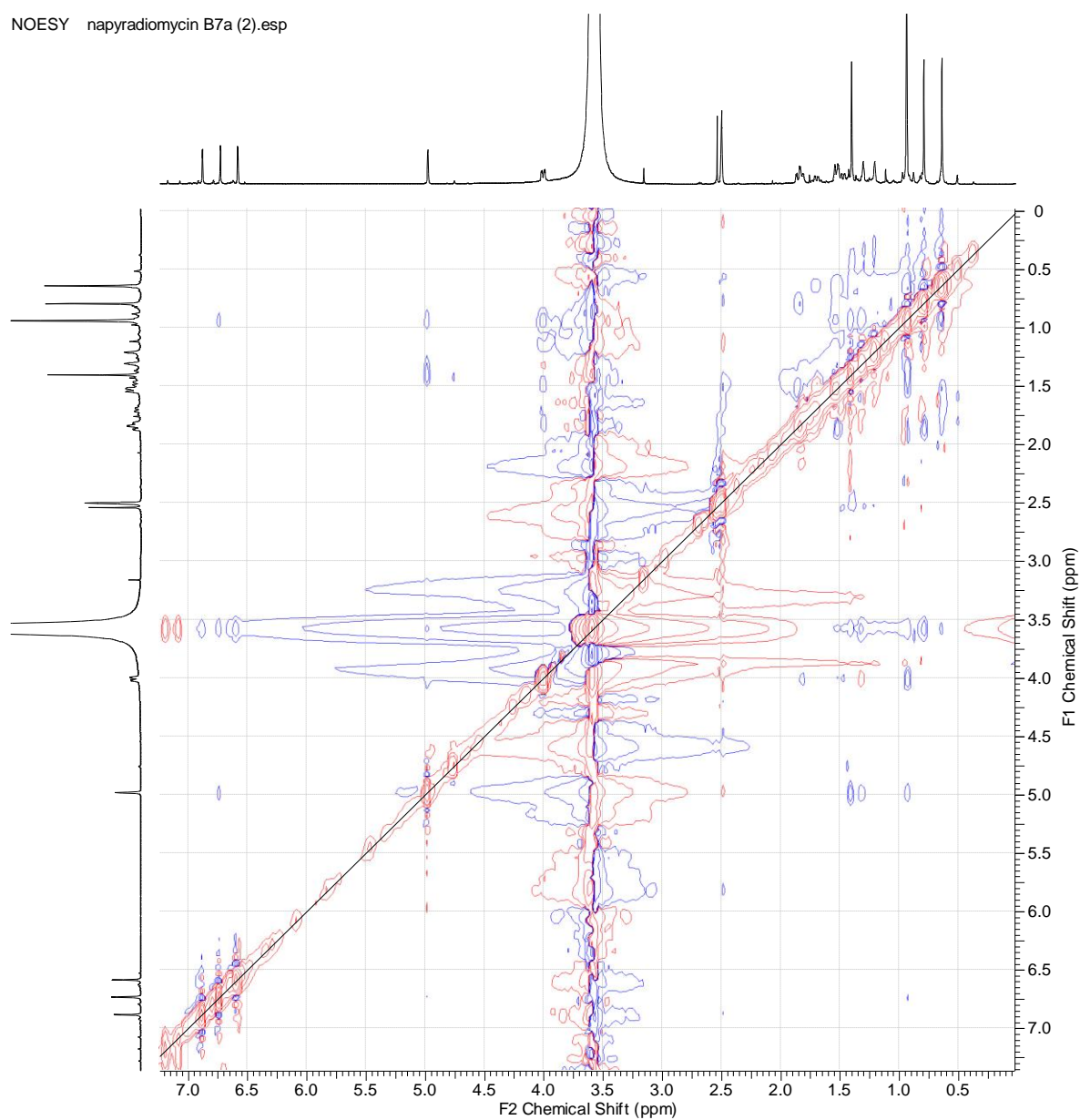


Figure S15. NOESY of compound 2.

ROESY napyradiomycin B7a (2).esp

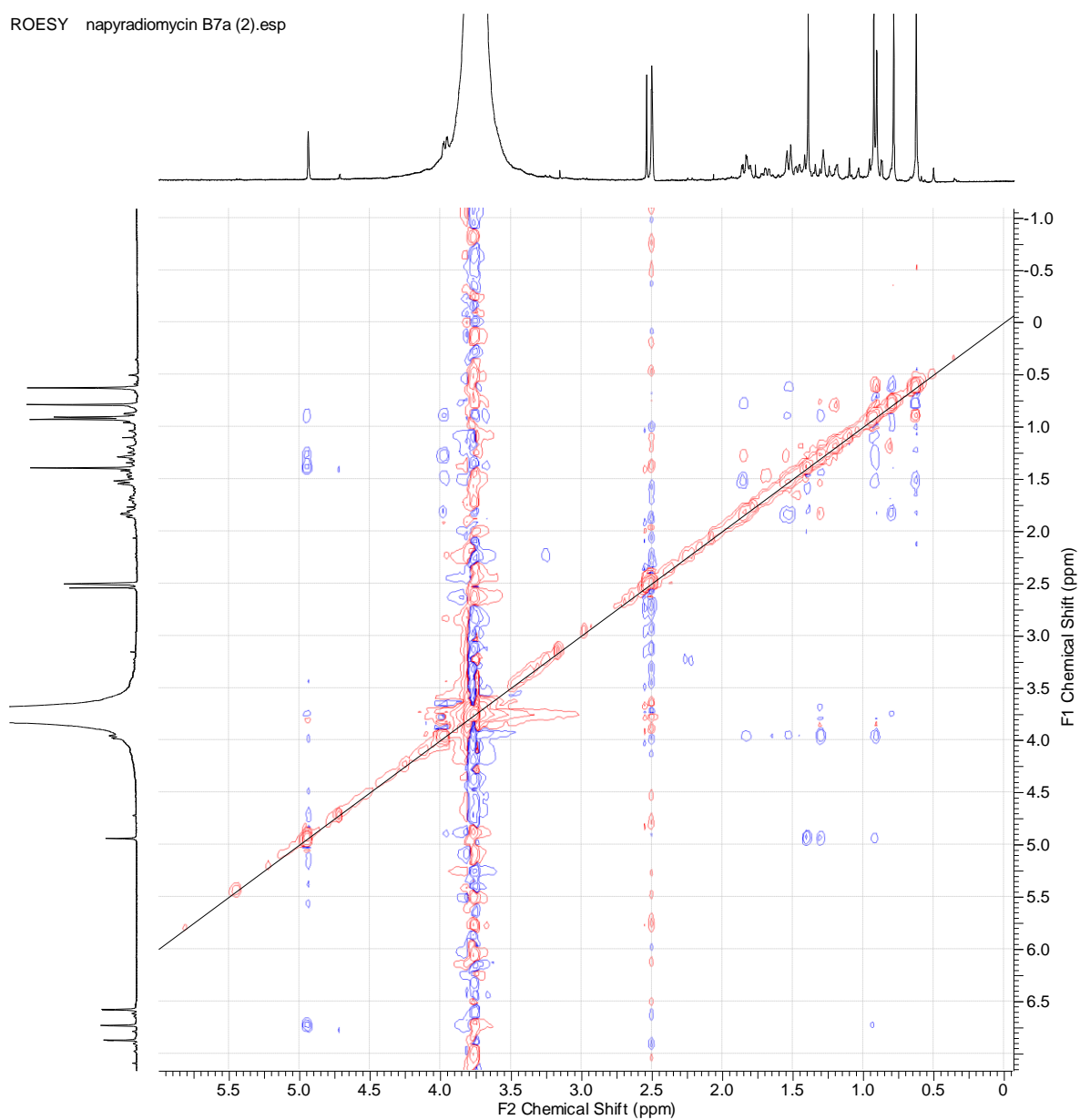


Figure S16. ROESY of compound 2.



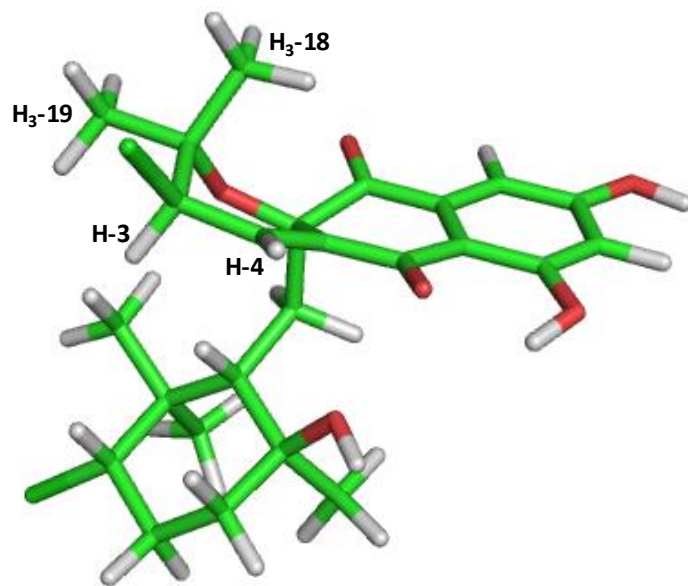
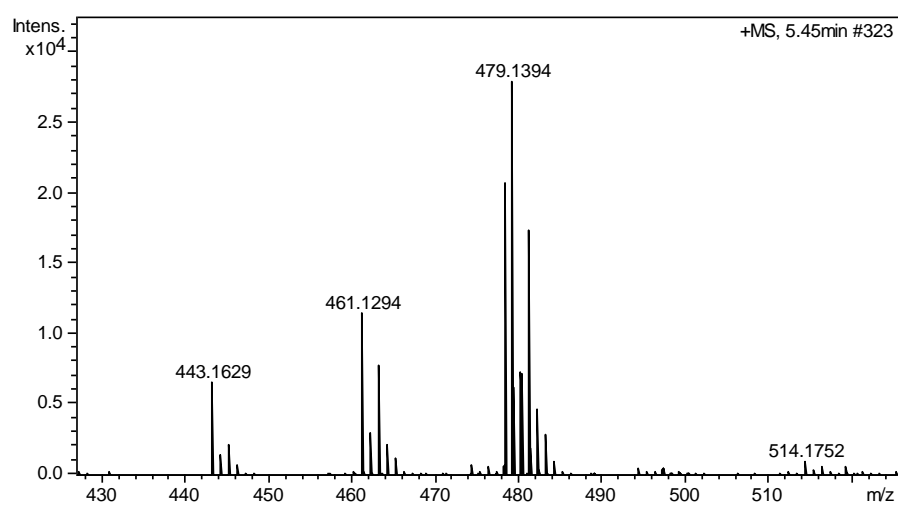
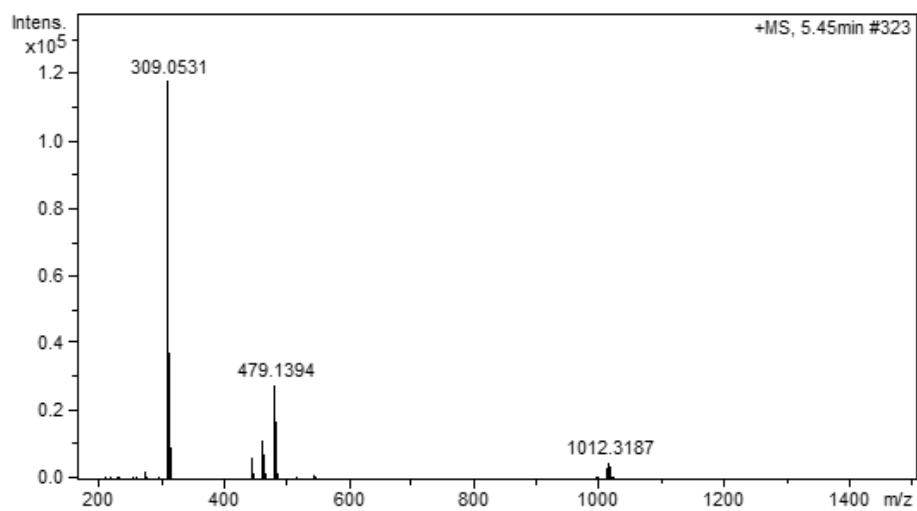
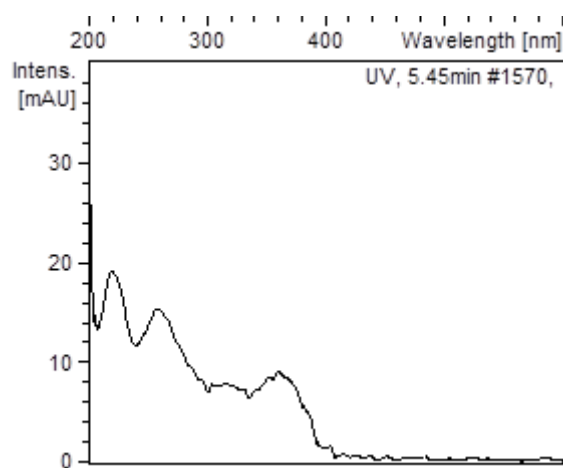


Figure S17. Energy minimized molecular model of compound 2.

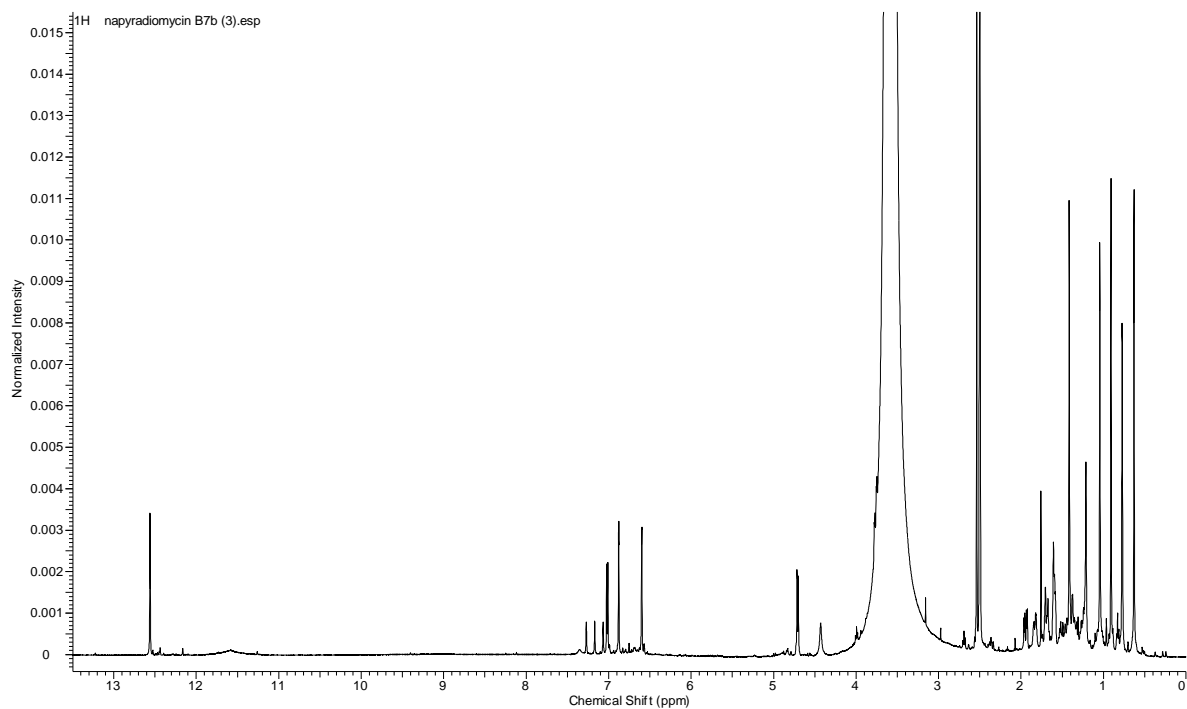


(A)

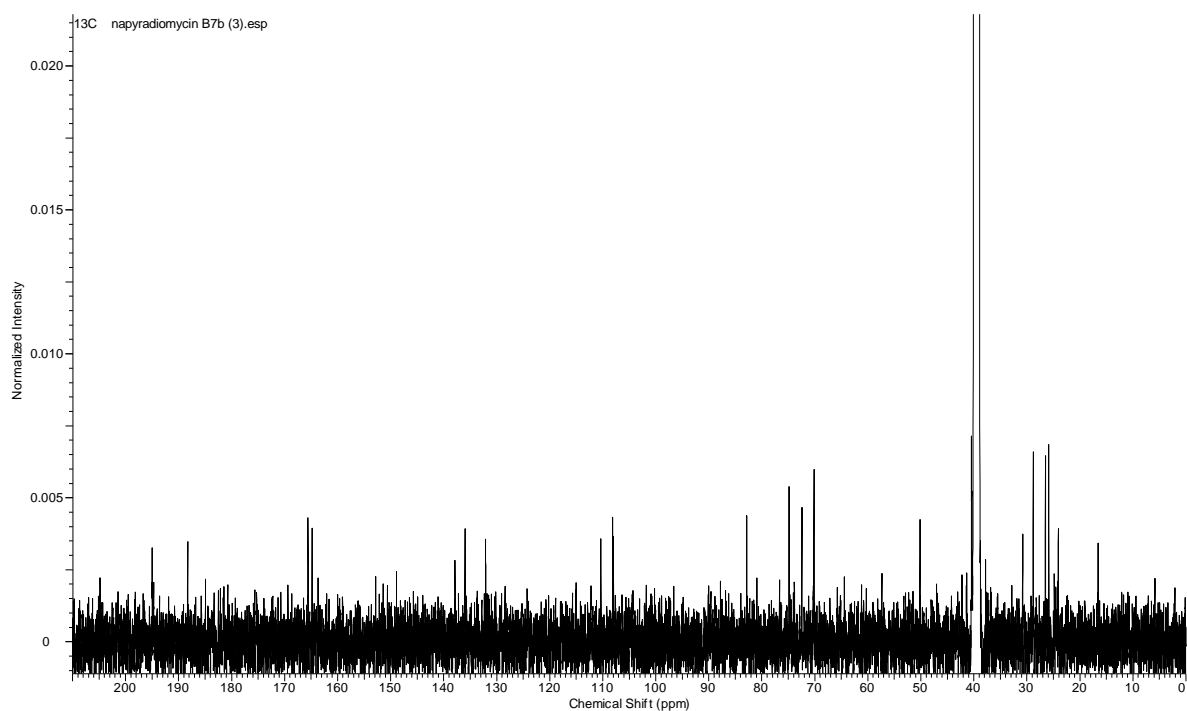


(B)

**Figure S18.** Electrospray-time of flight (ESI-TOF) (A) and UV (B) spectra of compound 3.

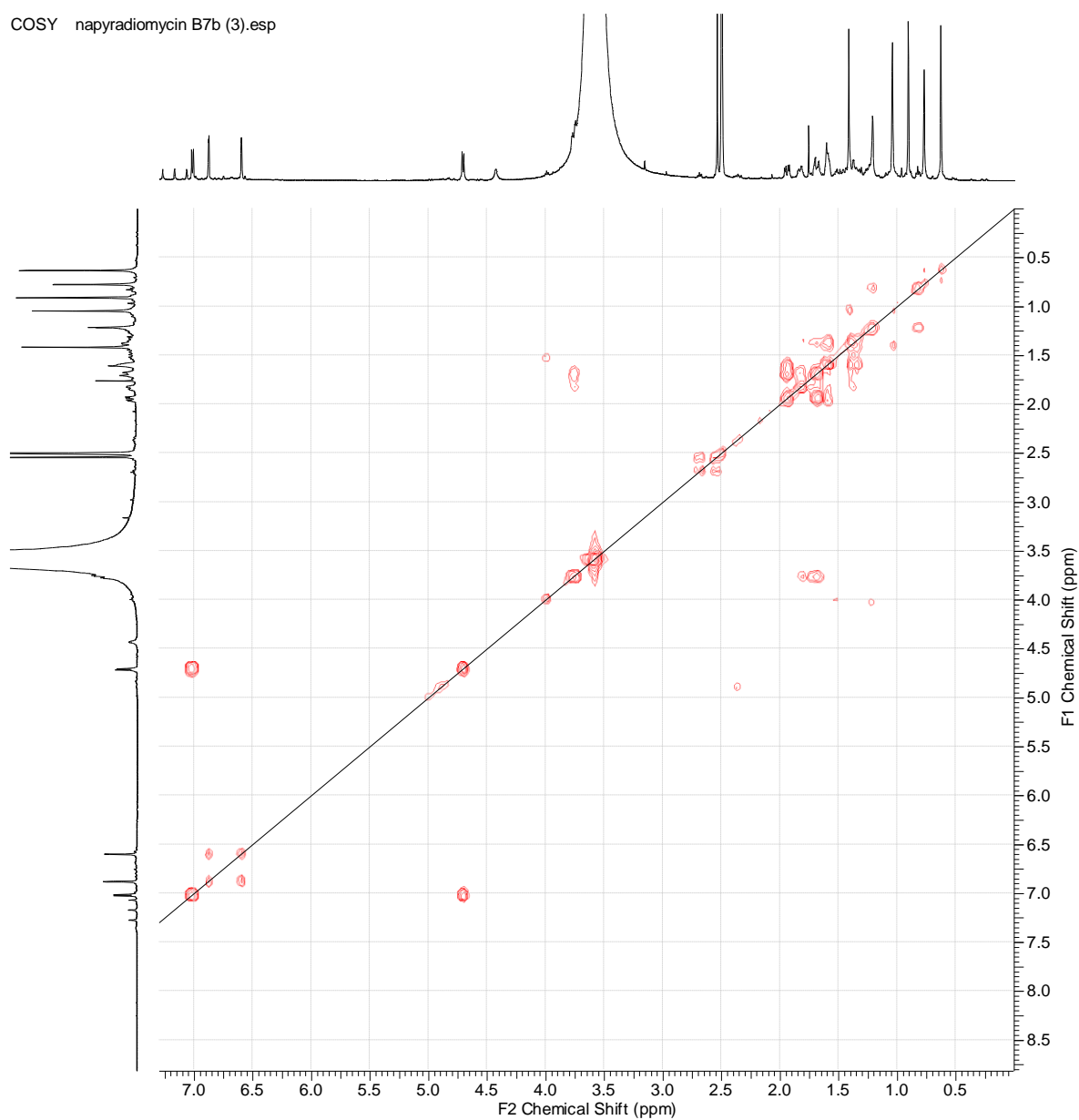


**Figure S19.** <sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 500 MHz) of compound 3.



**Figure S20.** <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 500 MHz) of compound 3.

COSY napyradiomycin B7b (3).esp

**Figure S21.** COSY of compound 3.

HSQC napyradiomycin B7b (3).esp

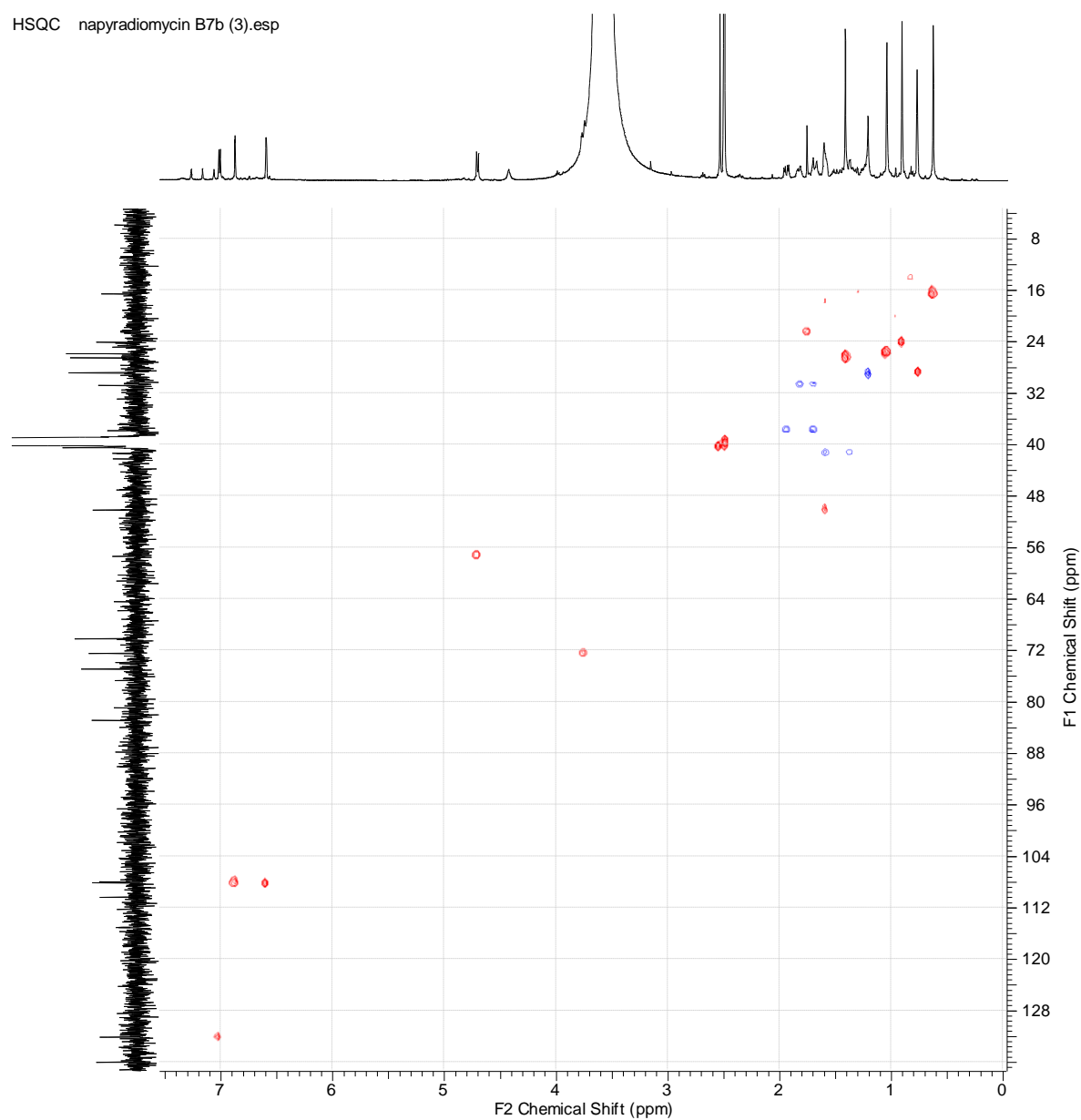


Figure S22. HSQC spectrum of compound 3.

HMBC napyradiomycin B7b (3).esp

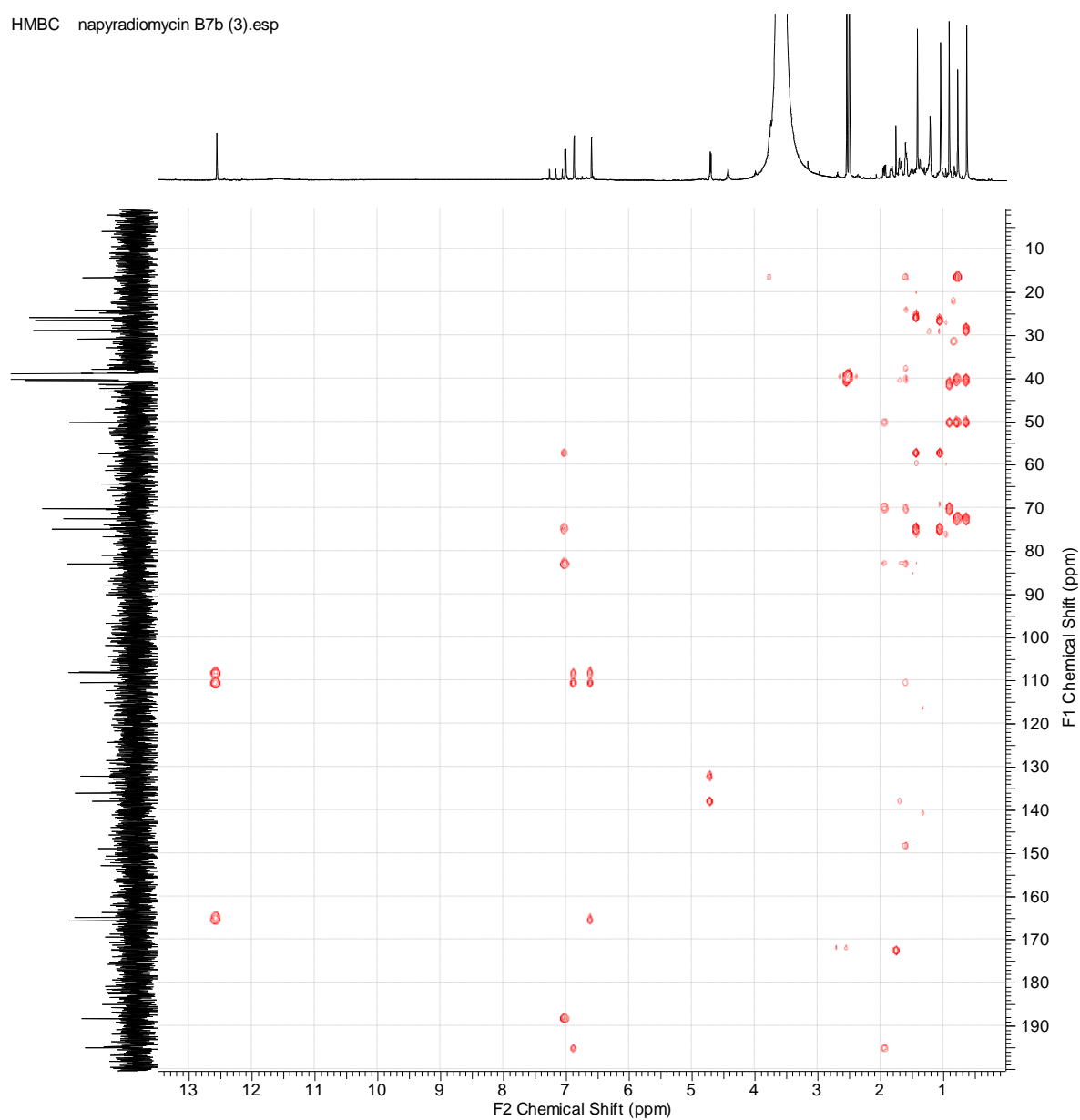


Figure S23. HMBC of compound 3.

NOESY napyradiomycin B7b (3).esp

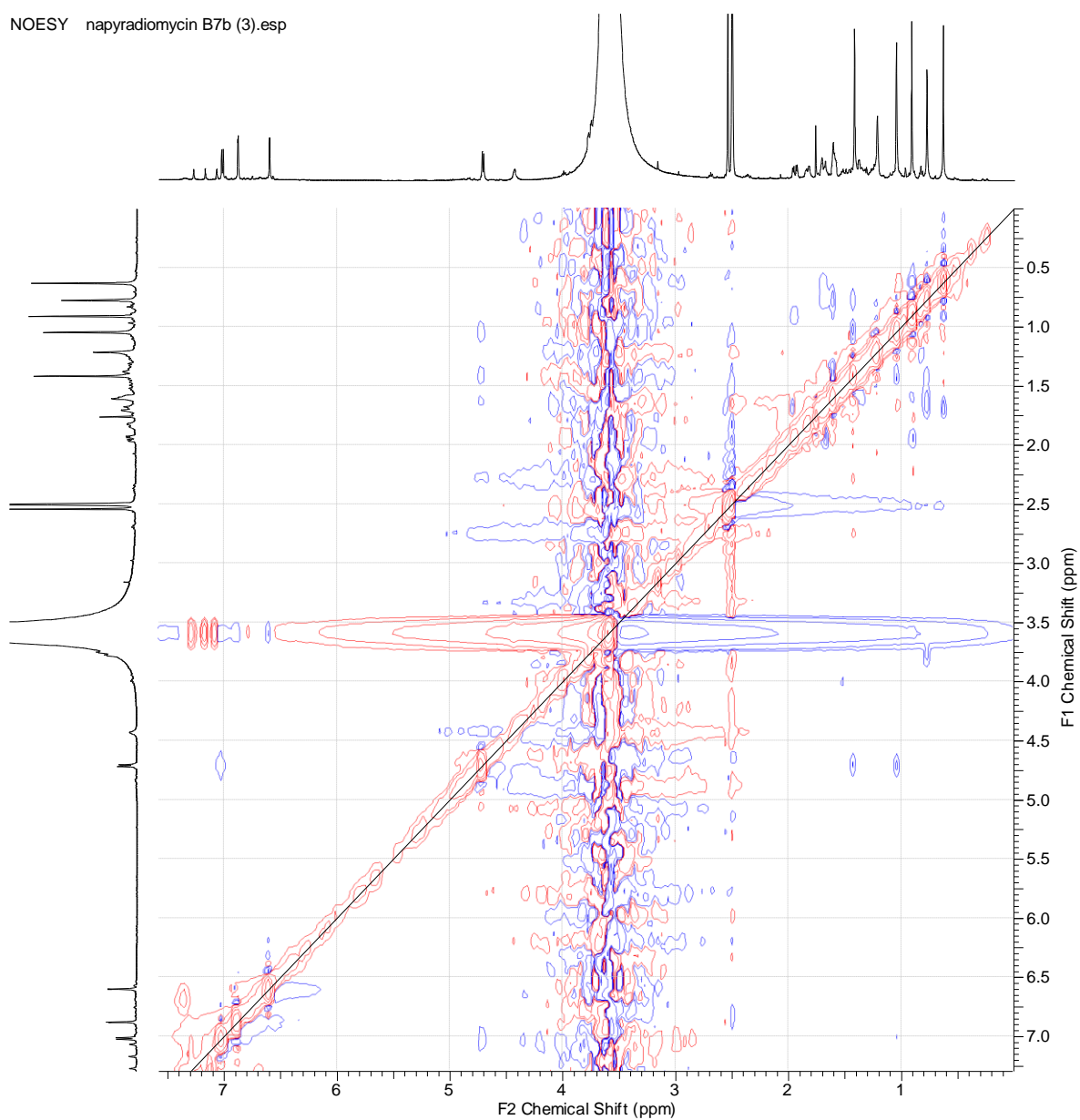


Figure S24. NOESY of compound 3.

ROESY napyradiomycin B7b (3).esp

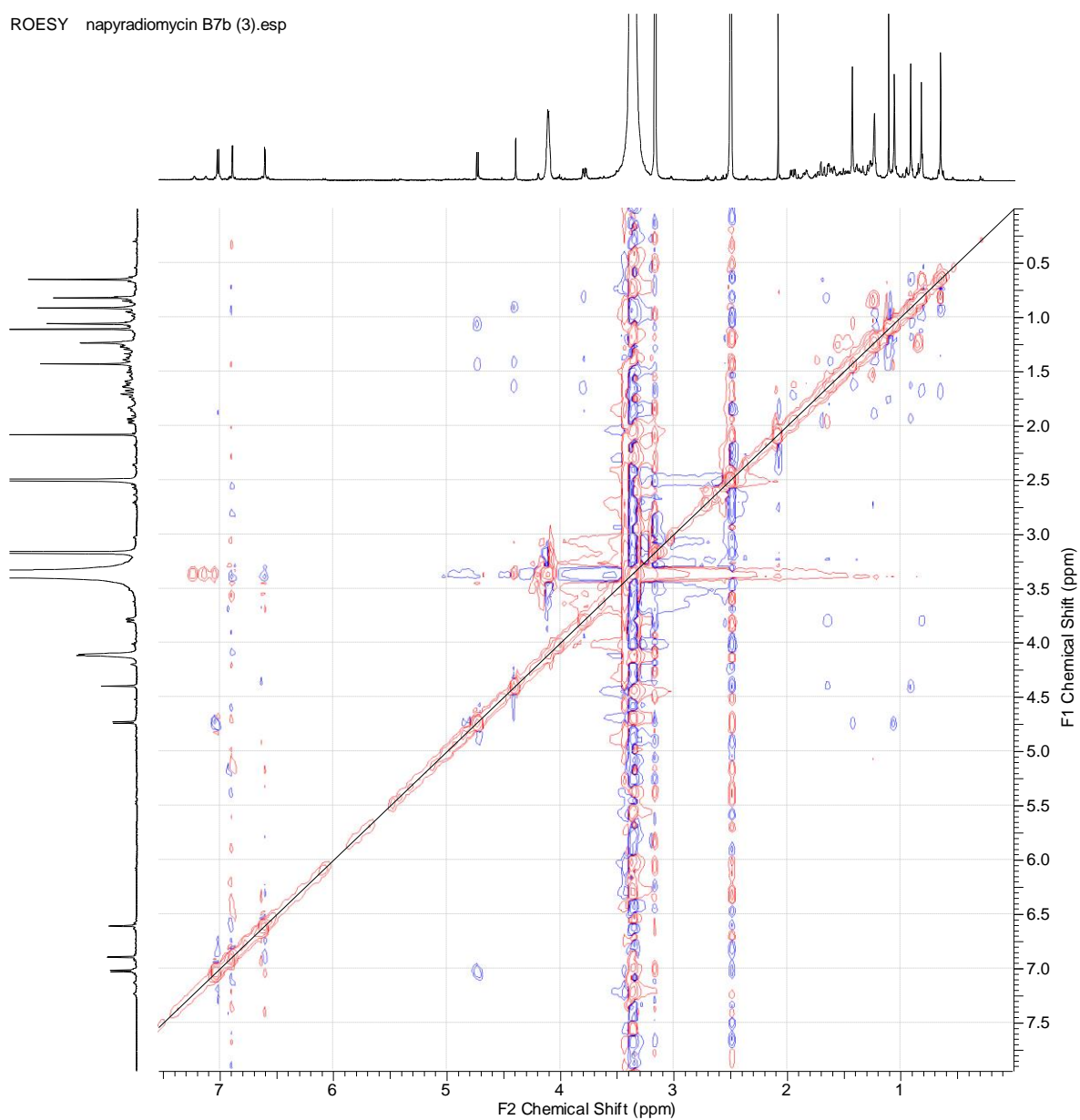


Figure S25. ROESY of compound 3.



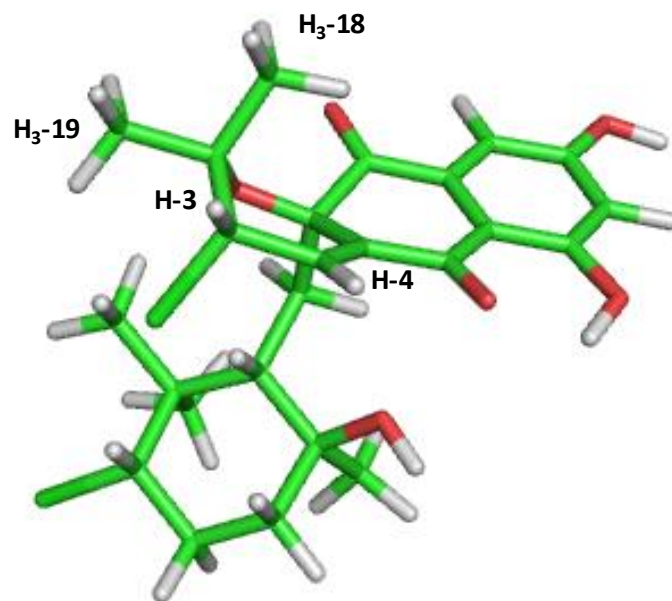
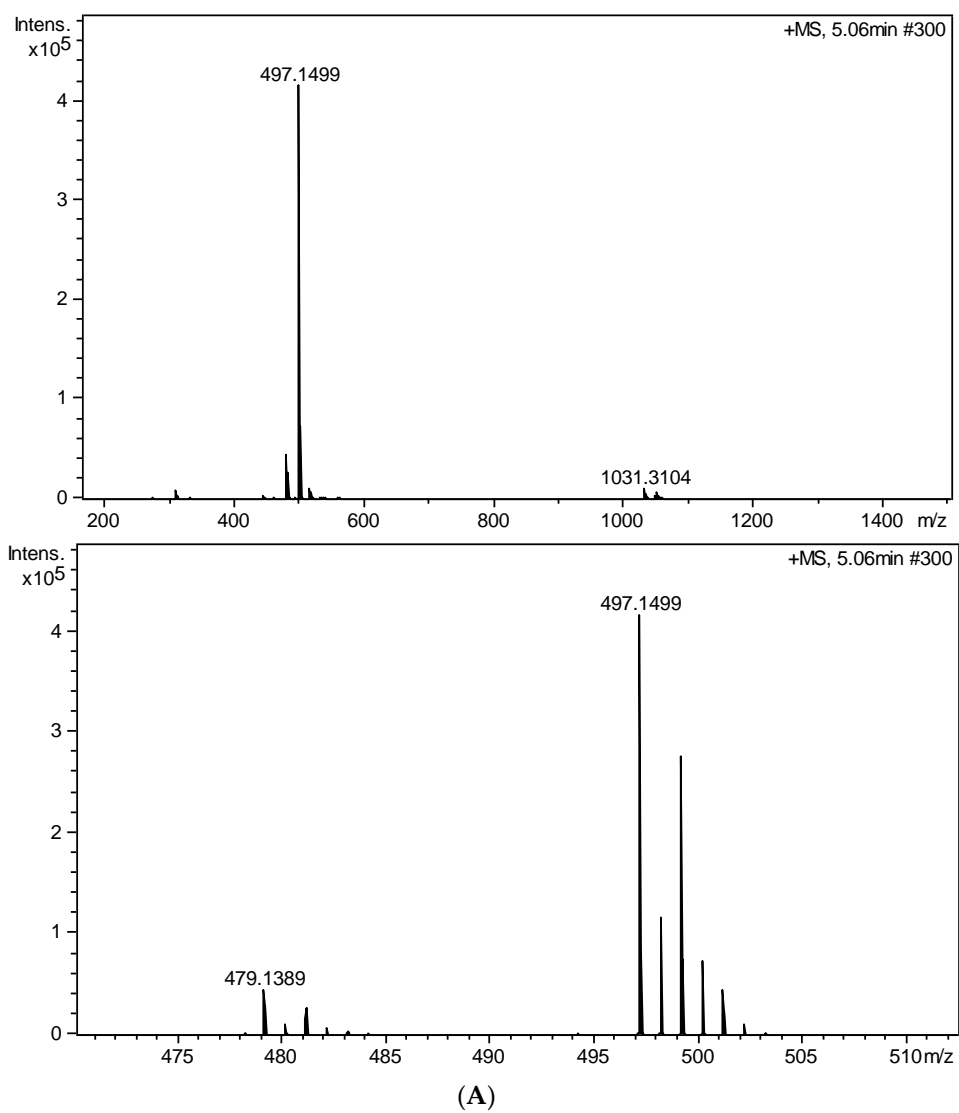
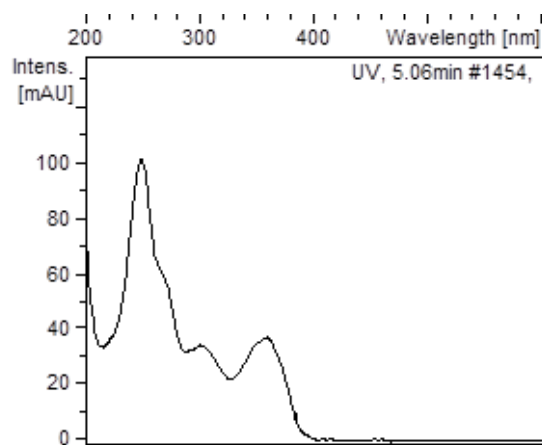


Figure S26. Energy minimized molecular model of compound 3.

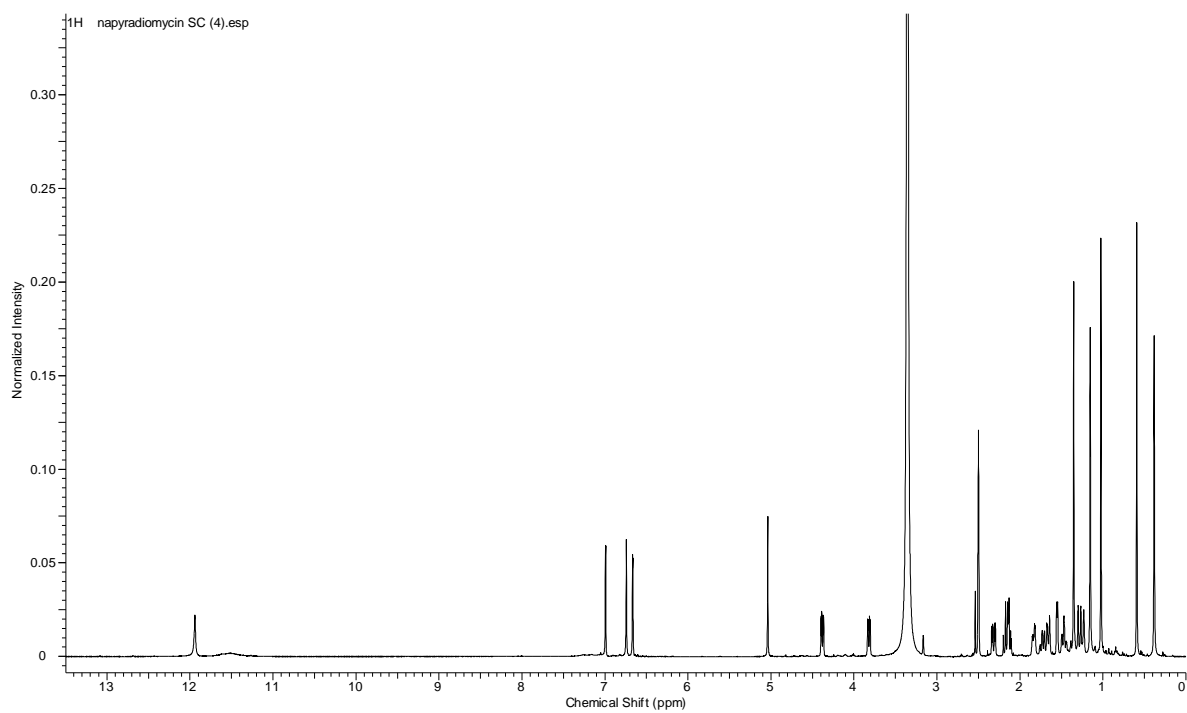


(A)

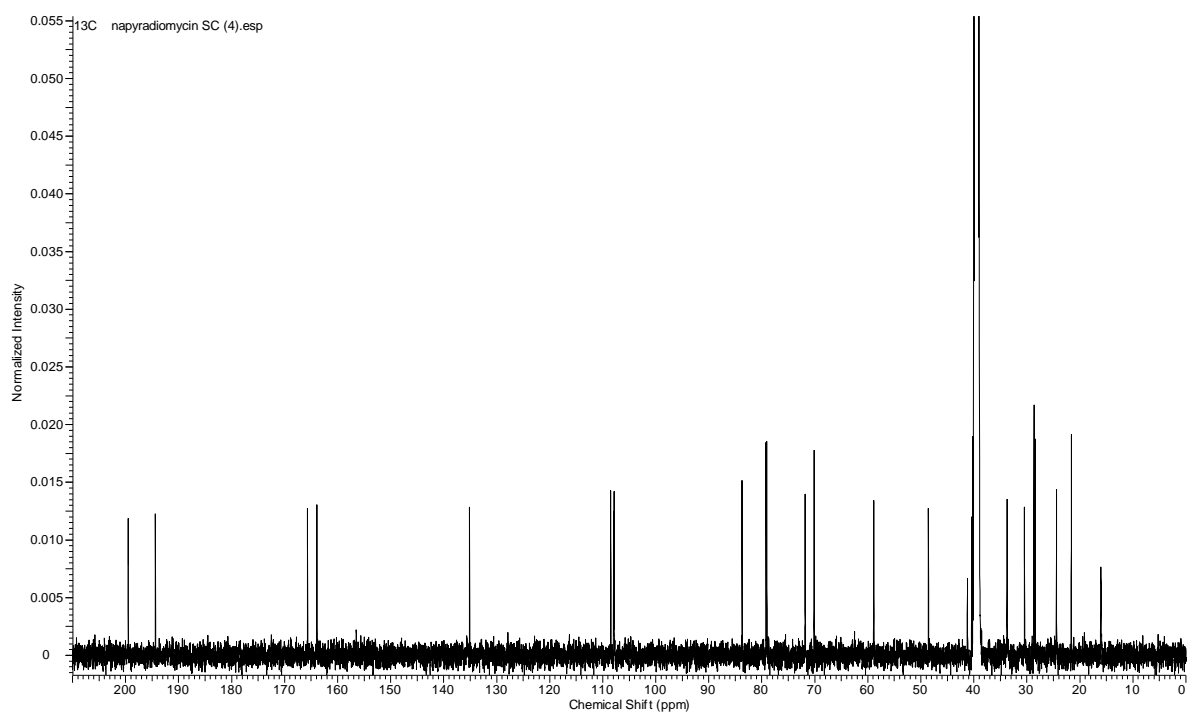


(B)

Figure S27. Electrospray-time of flight (ESI-TOF) (A) and UV (B) spectra of compound 4.

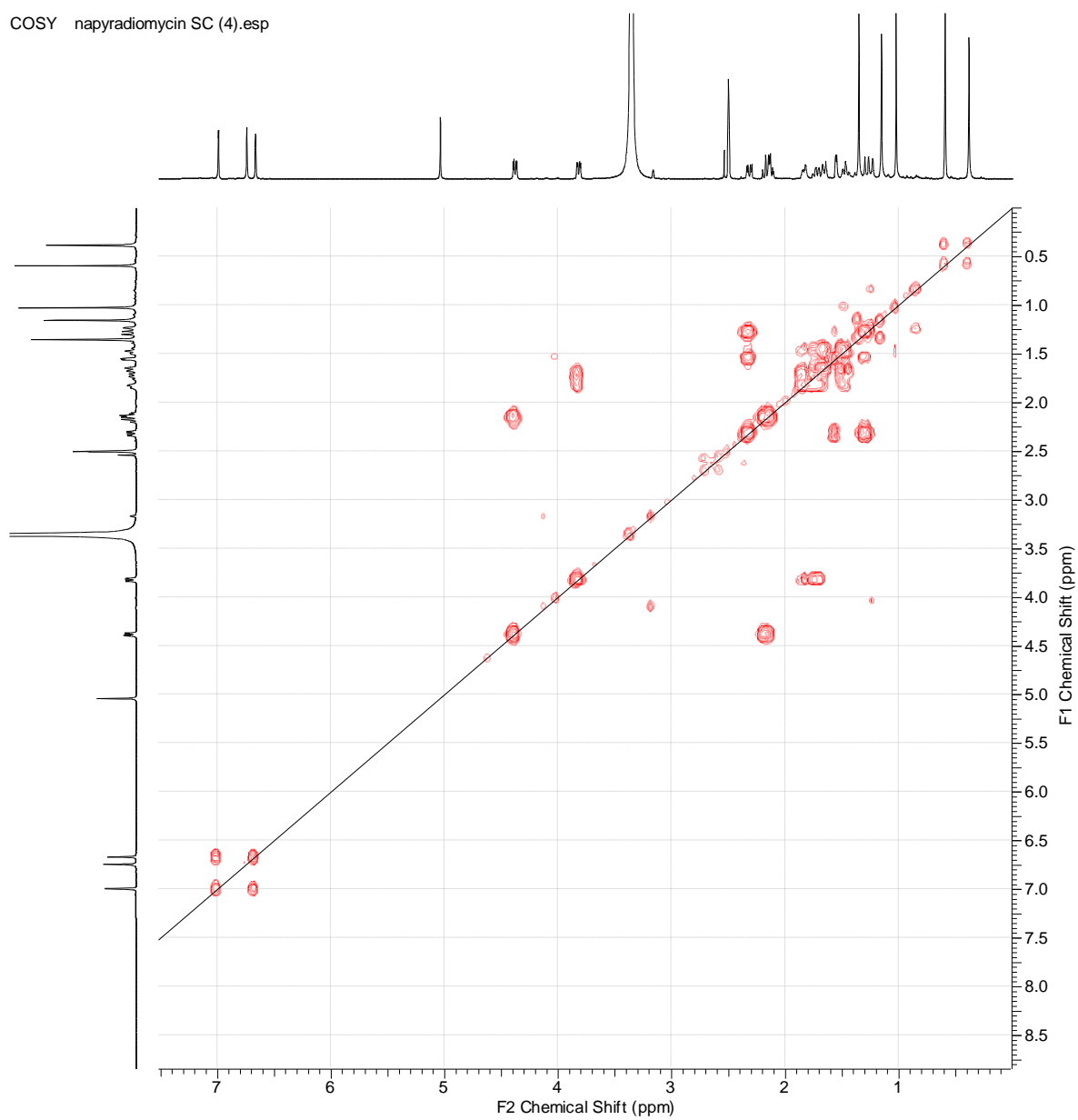


**Figure S28.** <sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 500 MHz) of compound 4.



**Figure S29.** <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 500 MHz) of compound 4.

COSY napradiomycin SC (4).esp

**Figure S30.** COSY of compound 4.

HSQC napyradiomycin SC (4).esp

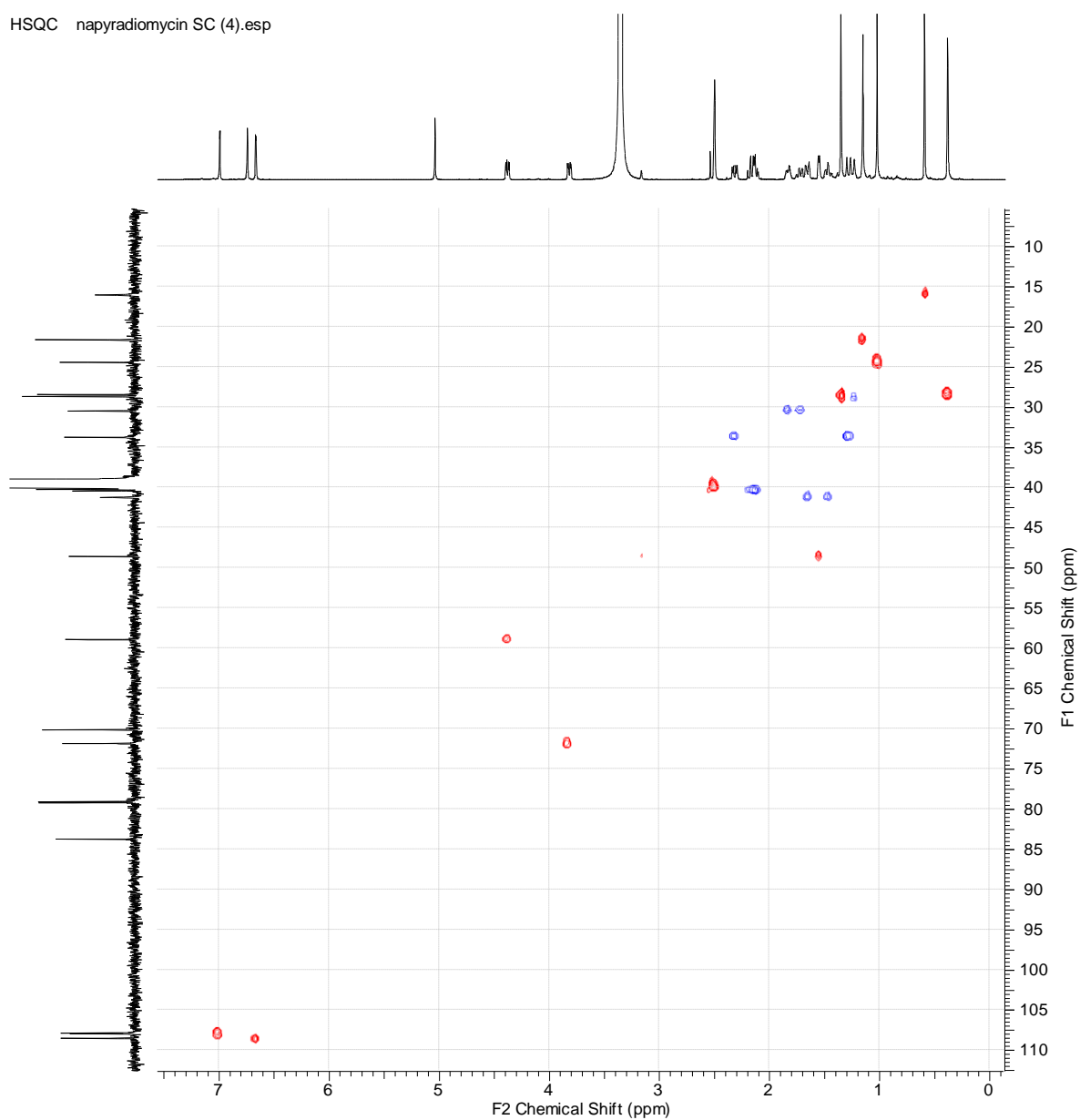


Figure S31. HSQC spectrum of compound 4.

HMBC napyradiomycin SC (4).esp

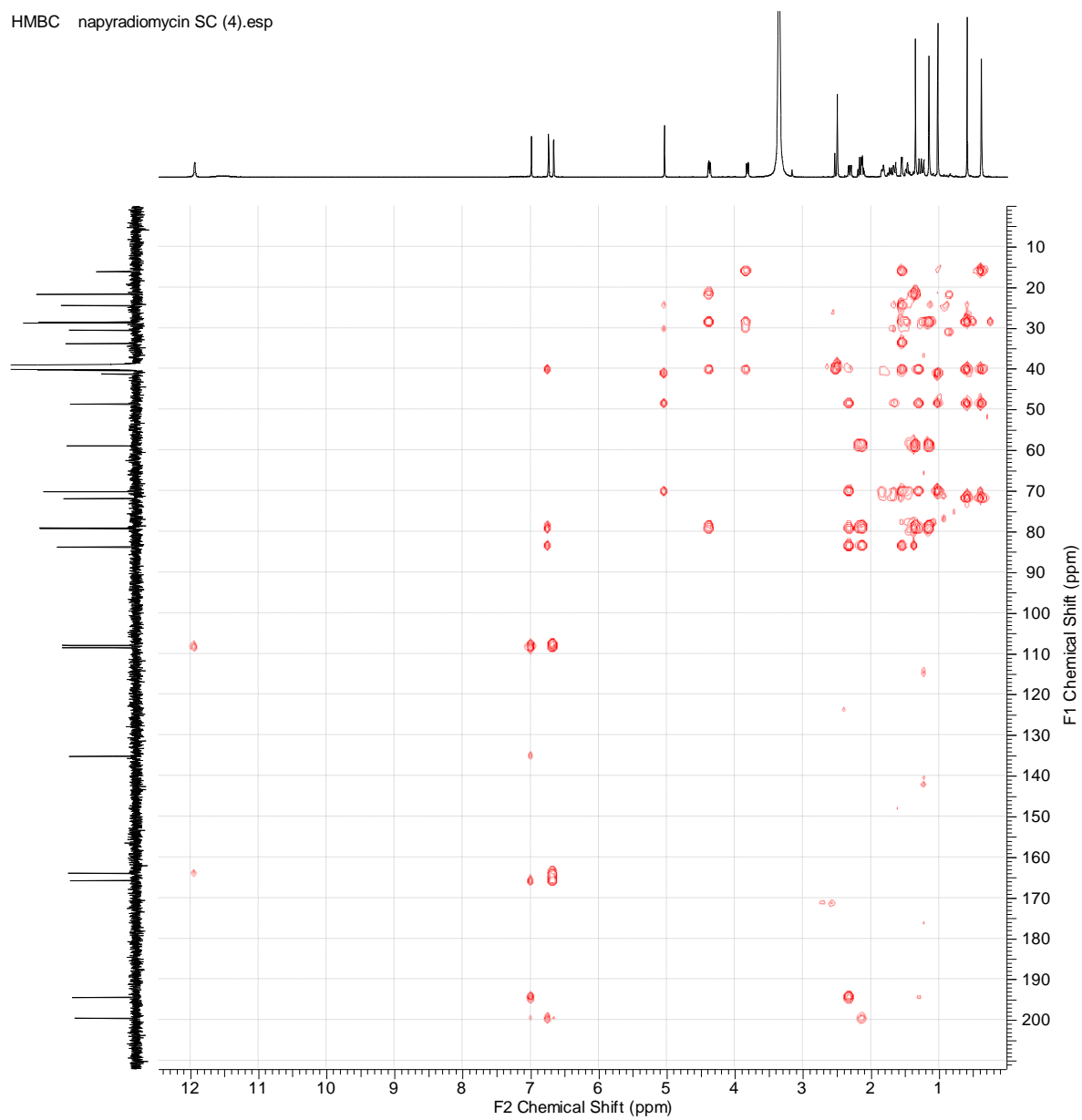


Figure S32. HMBC of compound 4.

NOESY napyradiomycin SC (4).esp

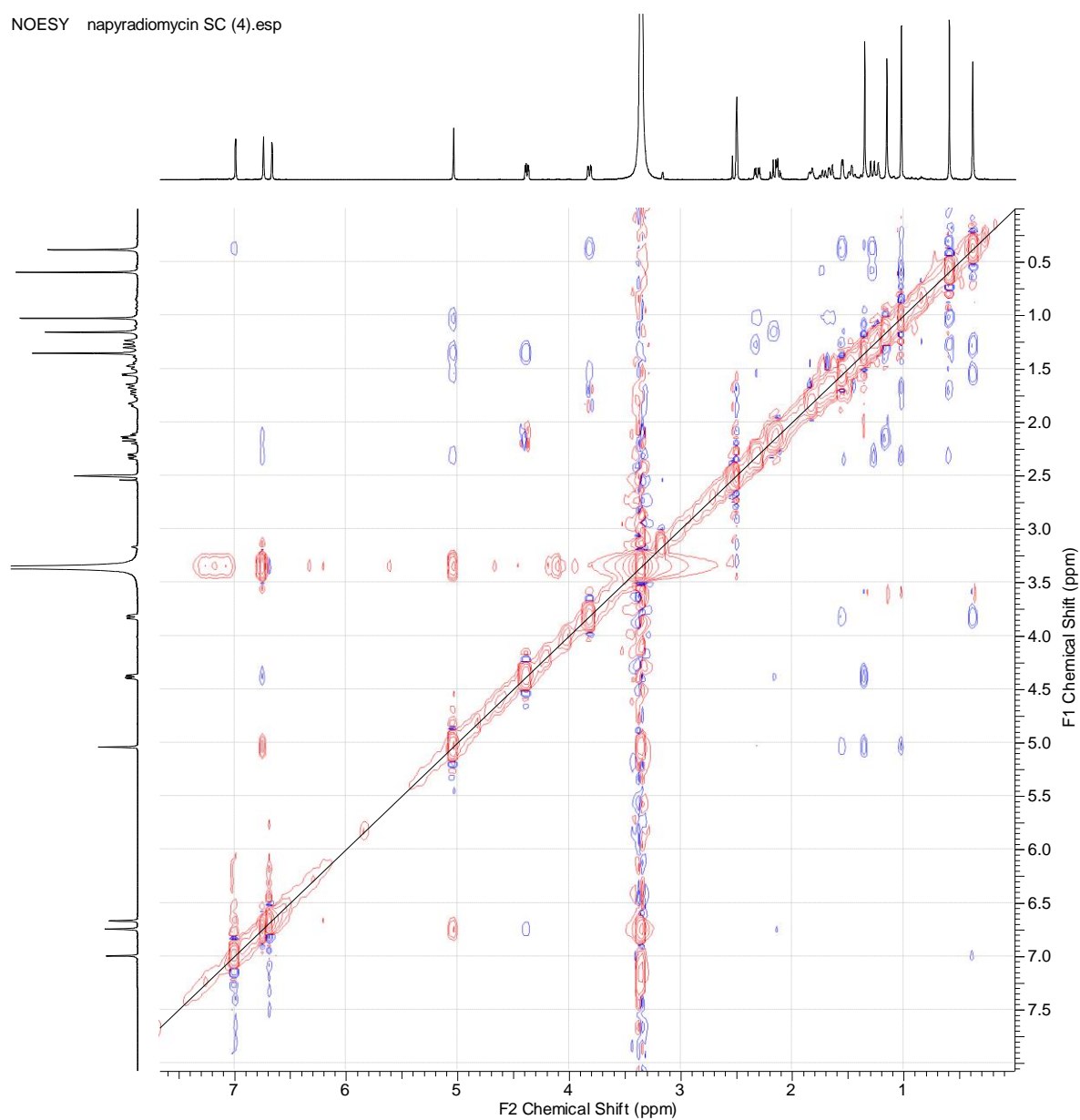


Figure S33. NOESY of compound 4.

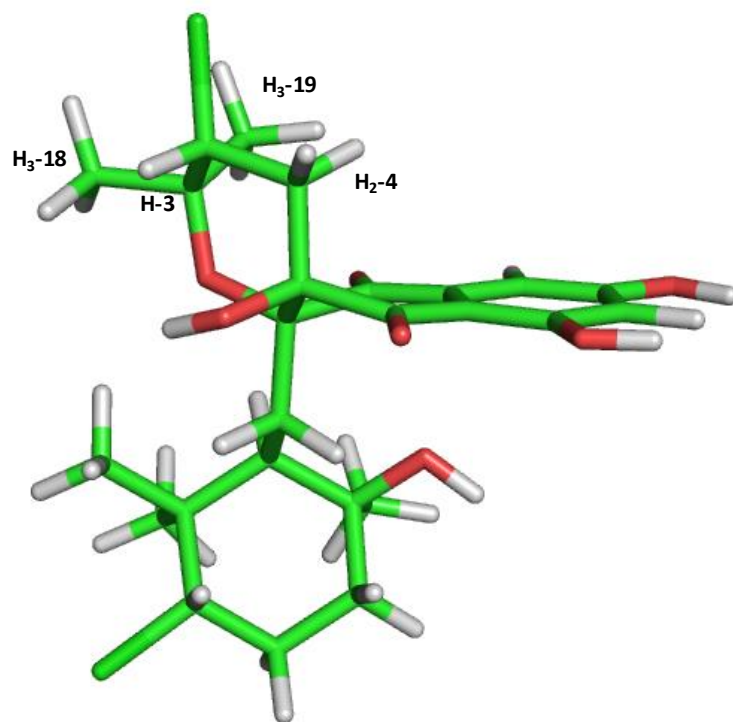


Figure S34. Energy minimized molecular model of compound 4.



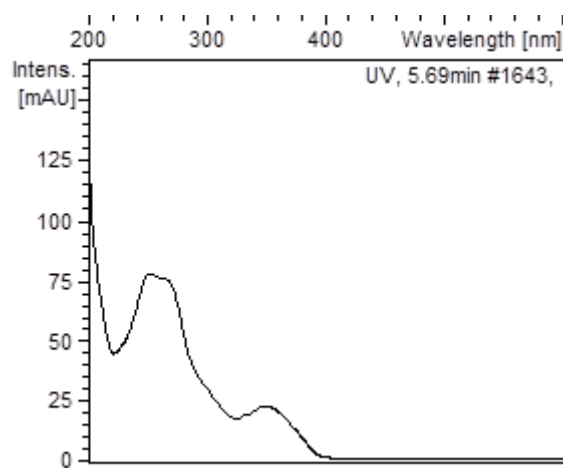
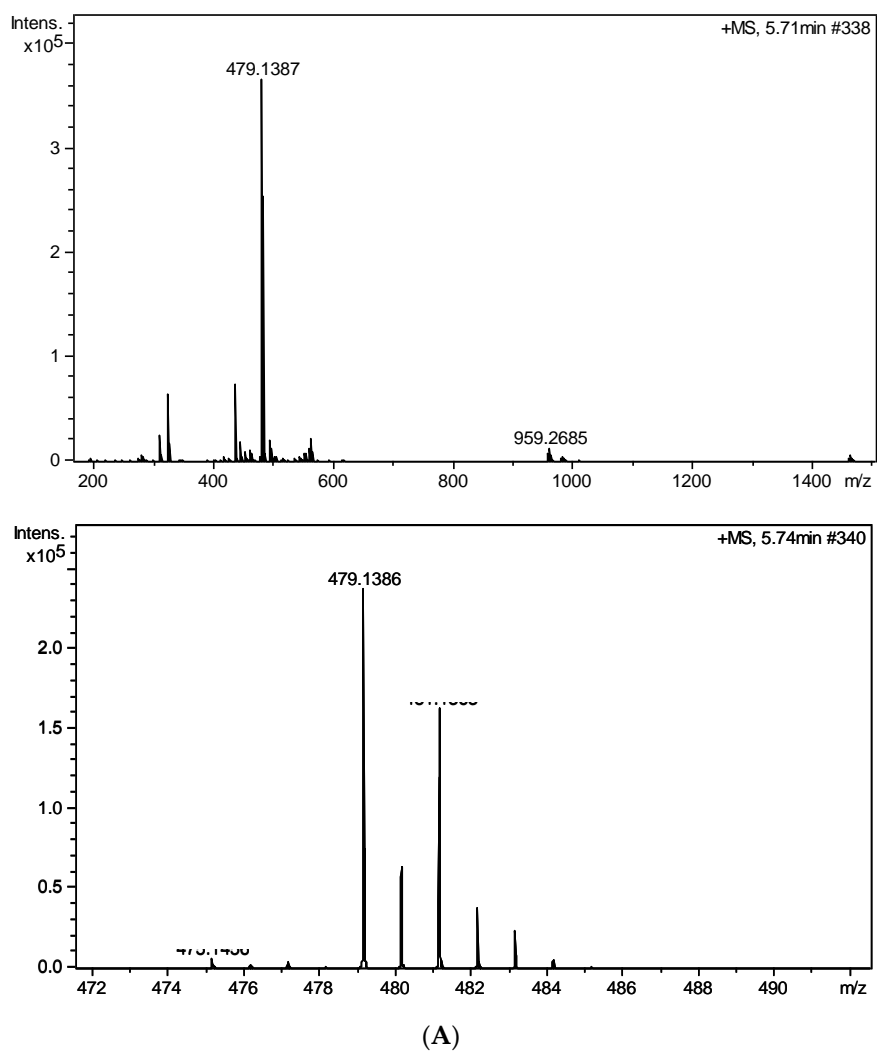


Figure S35. Electrospray-time of flight (ESI-TOF) (A) and UV (B) spectra of compound 5.

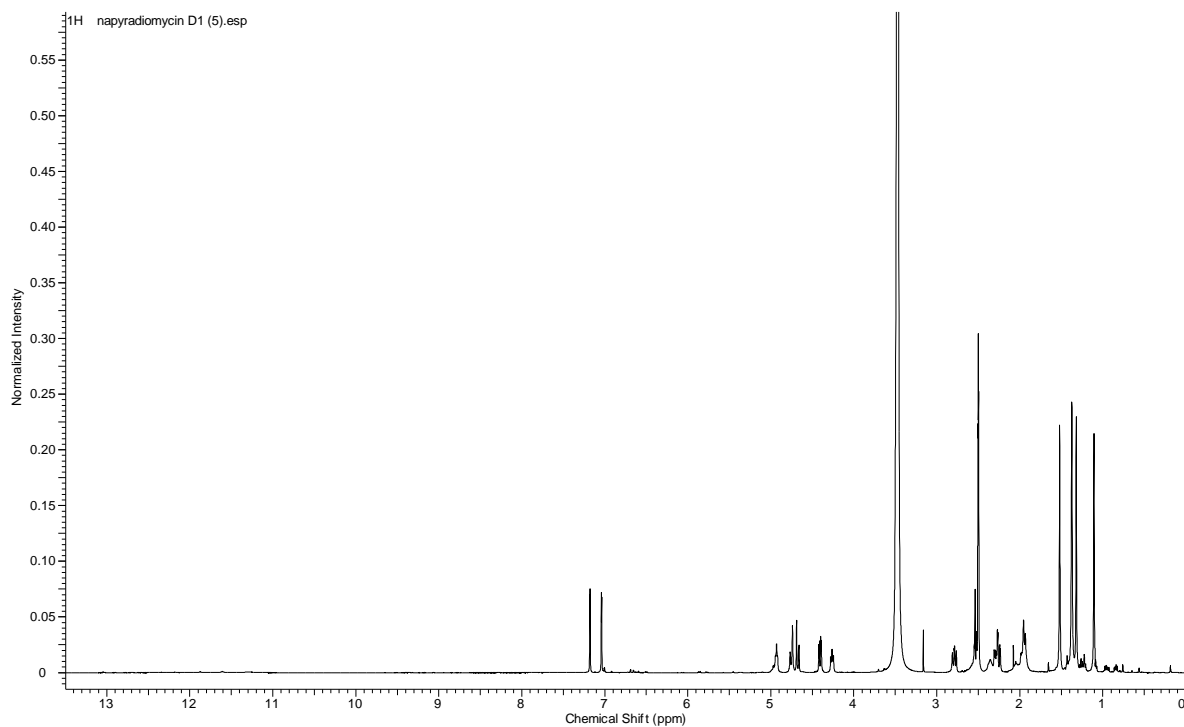


Figure S36. <sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 500 MHz) of compound 5.

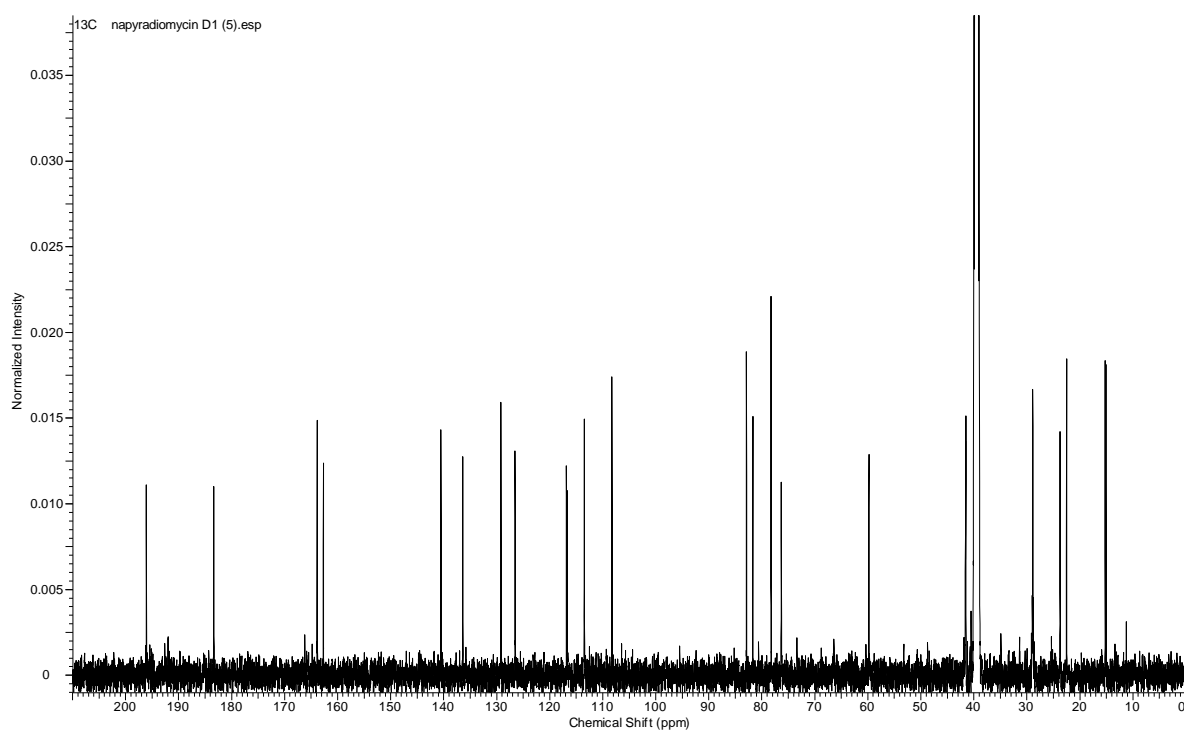


Figure S37. <sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 500 MHz) of compound 5.

COSY napradiomycin D1 (5).esp

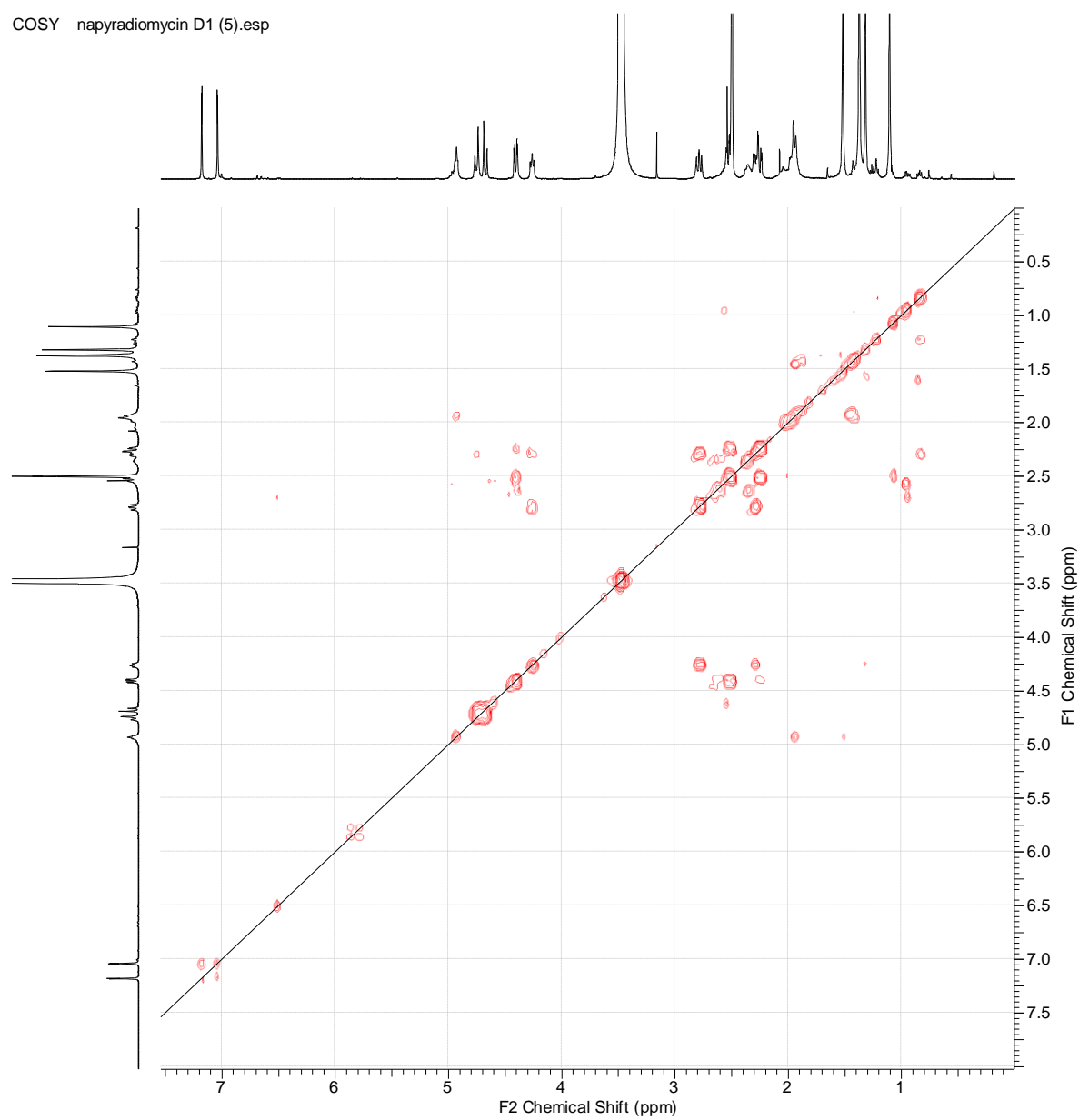


Figure S38. COSY of compound 5.

HSQC napyradiomycin D1 (5).esp

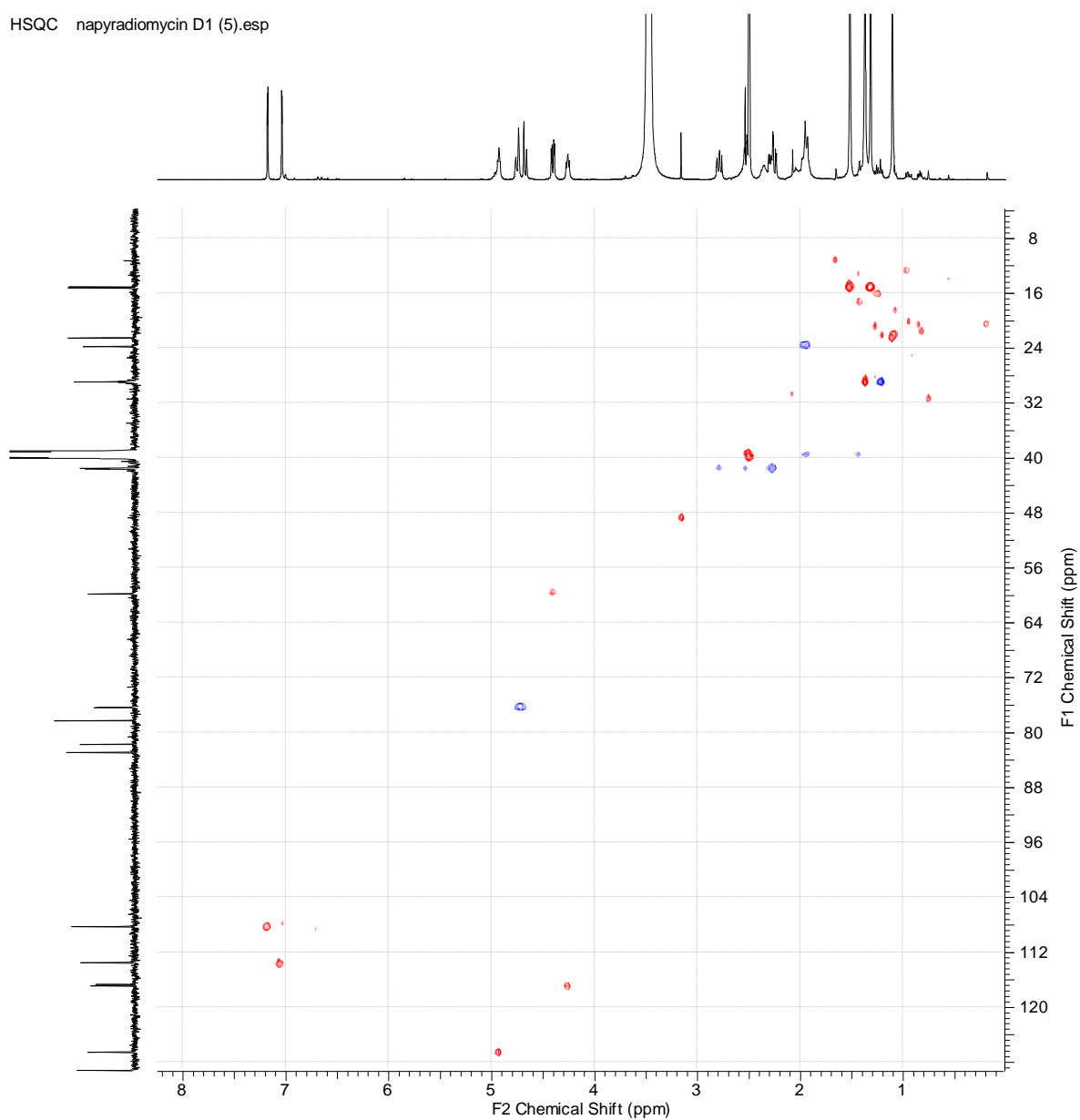
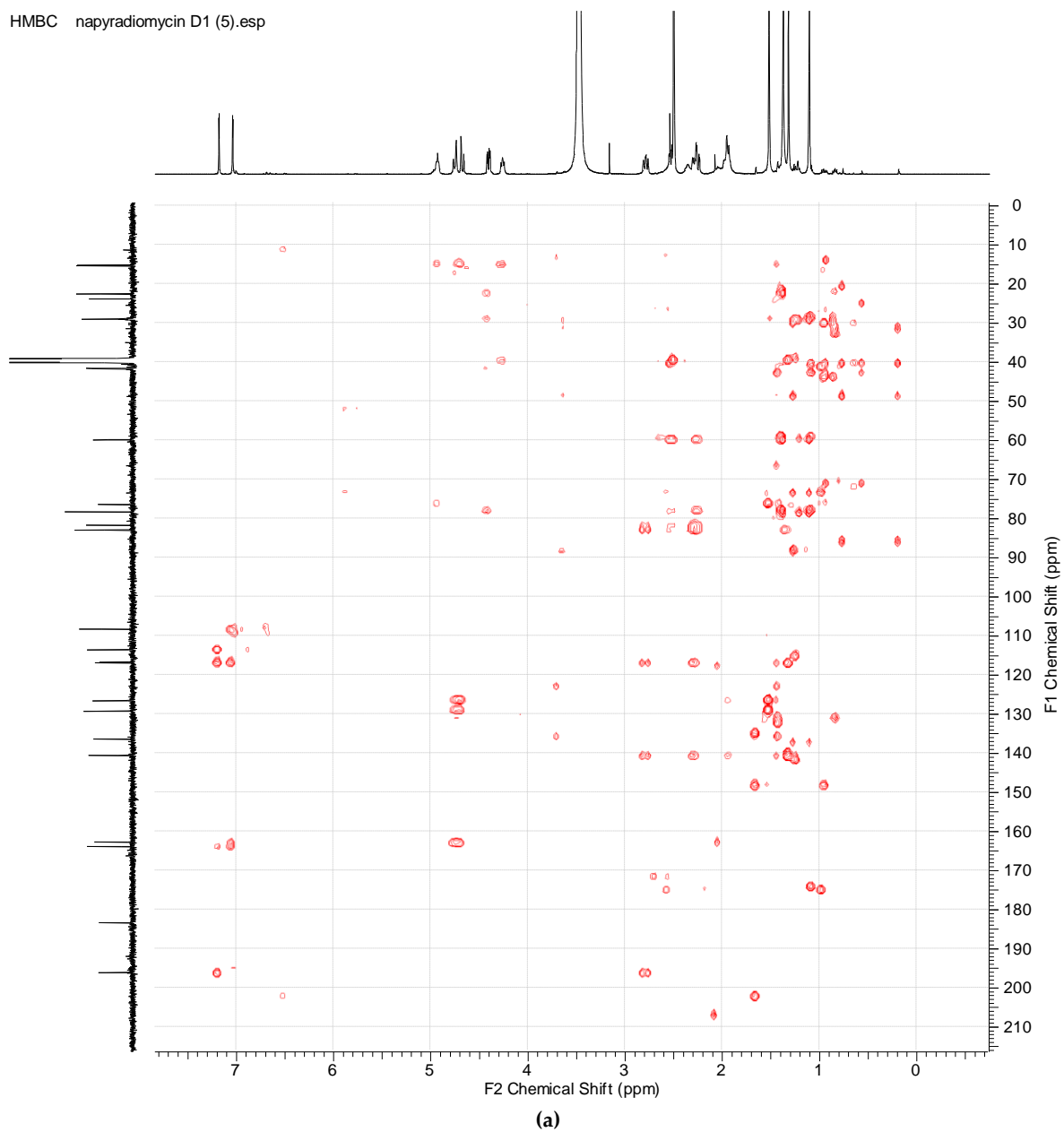
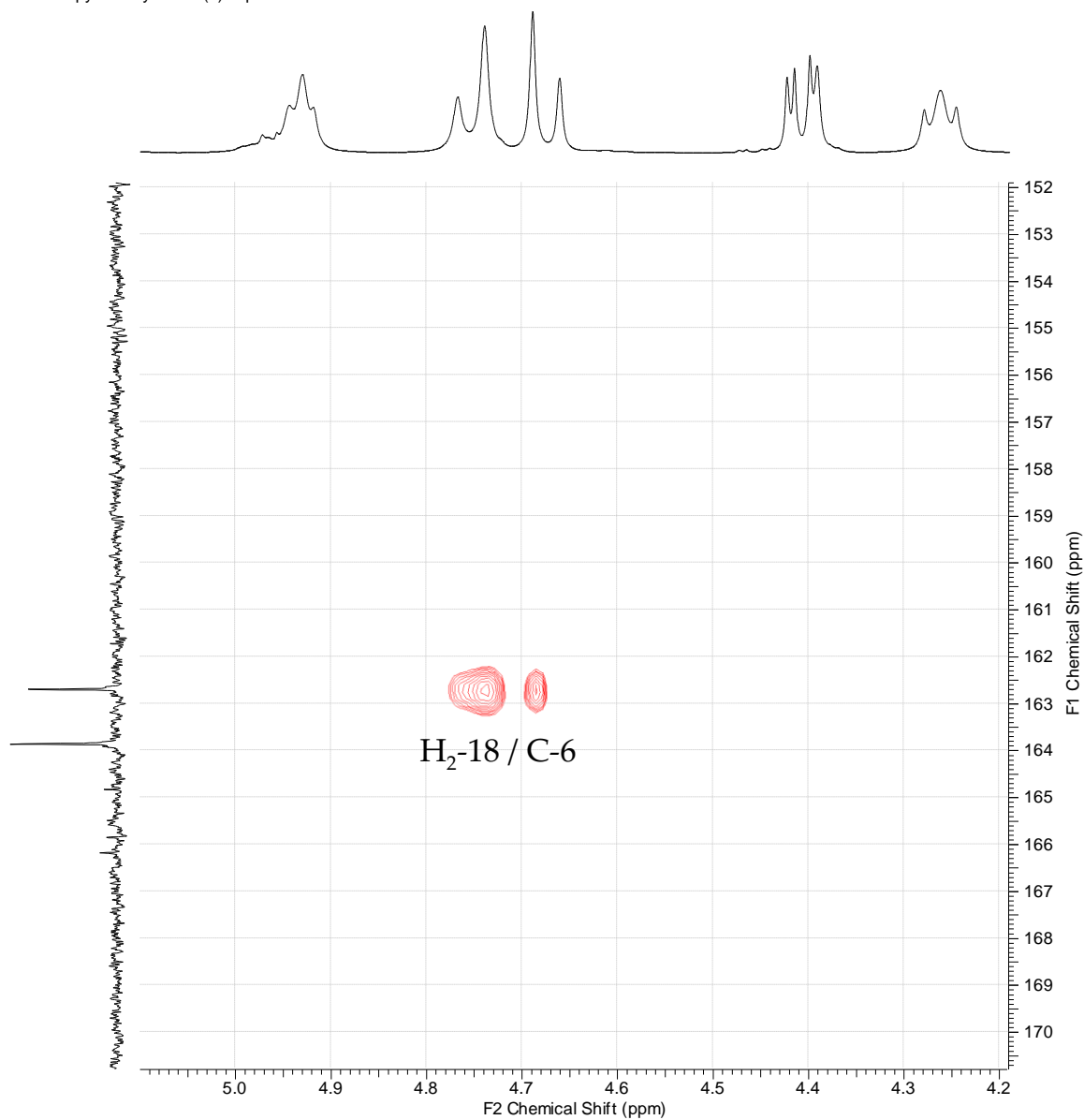


Figure S39. HSQC spectrum of compound 5.

HMBC napyradiomycin D1 (5).esp



HMBC napyradiomycin D1 (5).esp



(b)

**Figure S40.** (a) HMBC of compound 5. (b) Key HMBC correlation supporting the the etherification of the 18-hydroxy group in 5.

NOESY napradiomycin D1 (5).esp

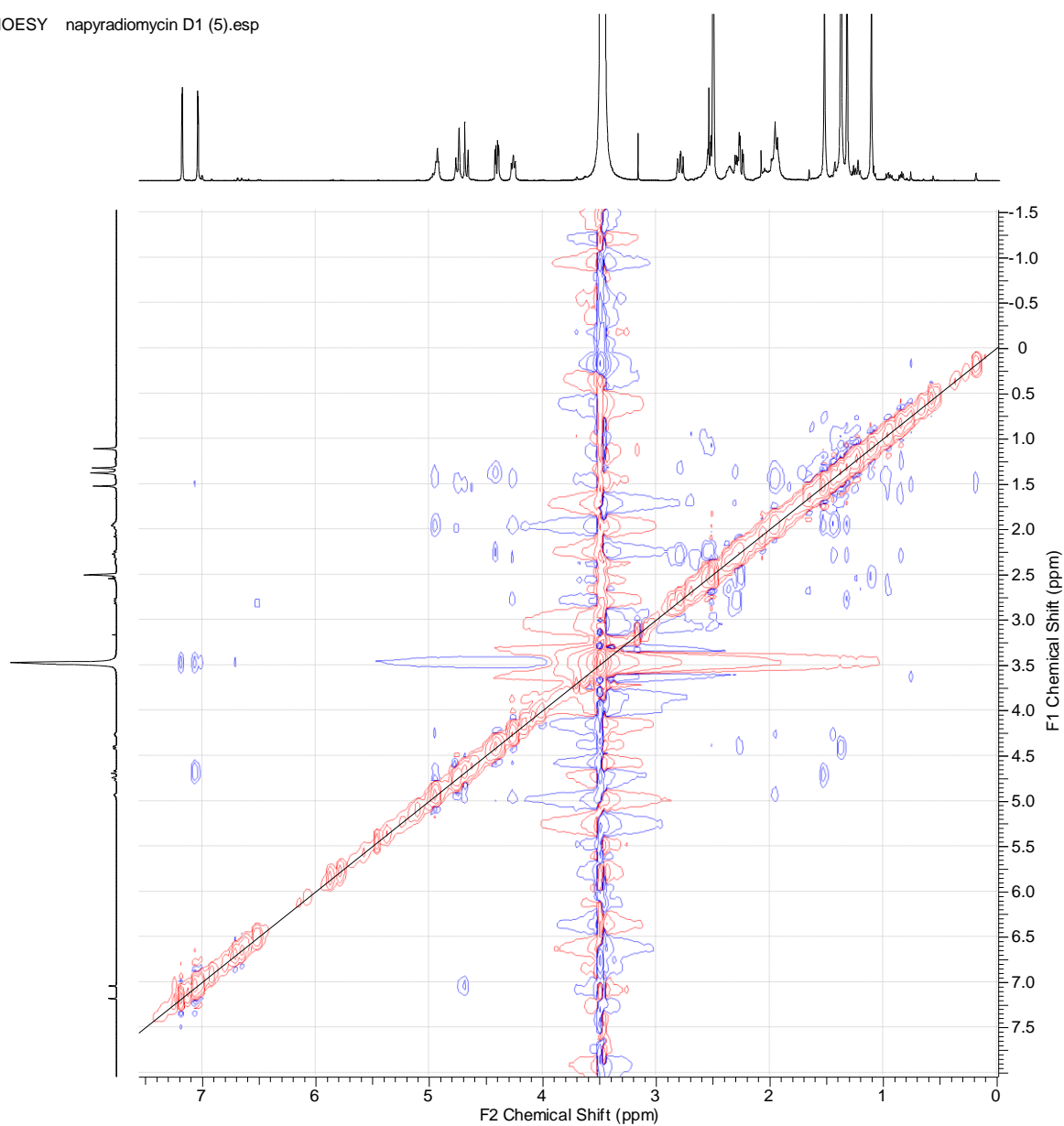


Figure S41. NOESY of compound 5.

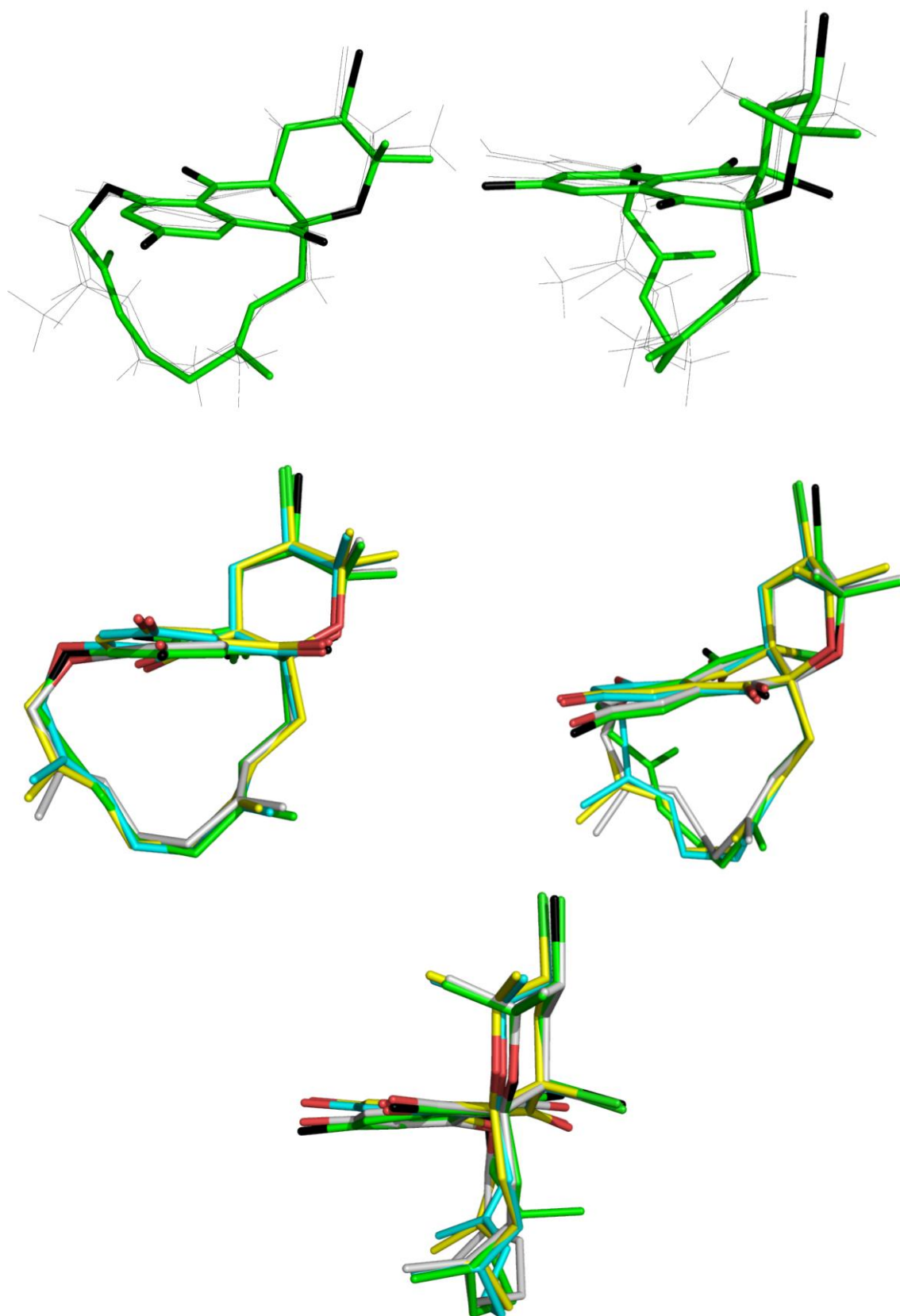


Figure S42. Overlay of different conformers for compound 5.



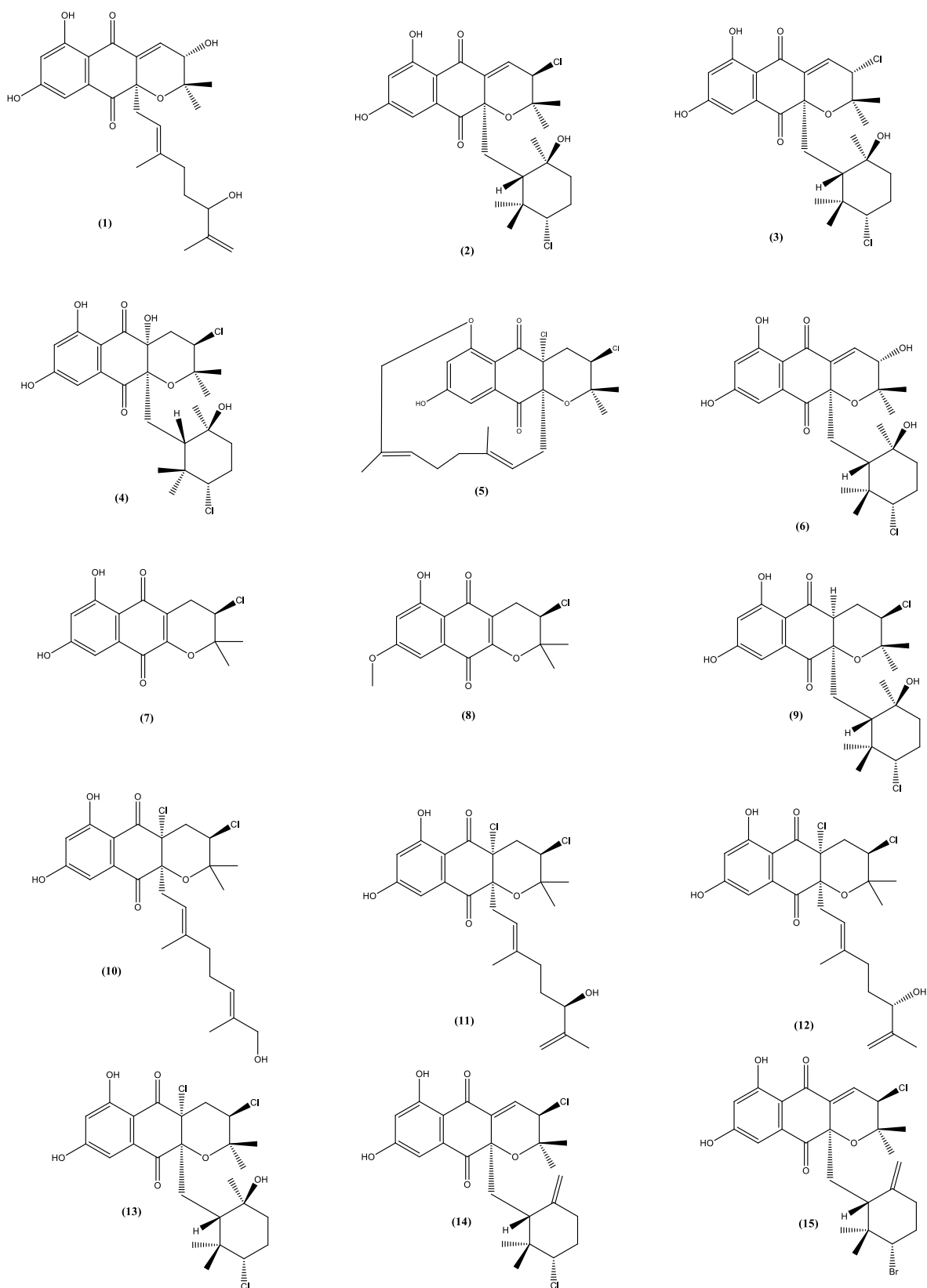


Figure S43. Napyradiomycins metabolites isolated from CA-271078 (1-15)