

Supplementary Information for

Anti-Parasitic Guanidine and Pyrimidine Alkaloids from the Marine Sponge***Monanchora arbuscula***

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- Page S3. Table S1. NMR Data (^1H 600 MHz, ^{13}C 150 MHz, ^{15}N , pyridine- d_5) for Batzellamide A (**8**).
Page S4. Table S2. NMR Data (^1H 600 MHz, ^{13}C 150 MHz, ^{15}N , DMSO- d_6) for Batzellamide A (**8**).
Page S5. Table S3. NMR Data (^1H 600 MHz, ^{13}C 150 MHz, ^{15}N , DMSO- d_6) for Hemibatzzelladines Δ^{19} (**10**) and Δ^{20} (**11**).
Page S6. Figure S1. ^1H NMR spectrum (600 MHz, DMSO- d_6) of monalidine A (**1**).
Page S7. Figure S2. ^{13}C NMR spectrum (150 MHz, DMSO- d_6) of monalidine A (**1**).
Page S8. Figure S3. gHSQC spectrum (DMSO- d_6) of monalidine A (**1**).
Page S9. Figure S4. COSY spectrum (DMSO- d_6) of monalidine A (**1**).
Page S10. Figure S5. gHMBC spectrum (DMSO- d_6) of monalidine A (**1**).
Page S11. Figure S6. tROESY spectrum (DMSO- d_6) of monalidine A (**1**).
Page S12. Figure S7. $^{15}\text{NLRHMQC}$ spectrum (DMSO- d_6) of monalidine A (**1**).
Page S13. Figure S8. ^1H NMR spectrum (400 MHz, DMSO- d_6) of 1-hydroxypentadecane-4,6-dione (**4**).
Page S14. Figure S9. ^{13}C NMR spectrum (100 MHz, DMSO- d_6) of 1-hydroxypentadecane-4,6-dione (**4**).
Page S15. Figure S10. ^1H NMR spectrum (400 MHz, CDCl_3) of 3-(2-imino-6-nonyl-2,3-dihydropyrimidin-4-yl)propan-1-ol (**6**).
Page S16. Figure S11. ^{13}C NMR spectrum (100 MHz, CDCl_3) of 3-(2-imino-6-nonyl-2,3-dihydropyrimidin-4-yl)propan-1-ol (**6**).
Page S17. Figure S12. ^1H NMR spectrum (400 MHz, DMSO- d_6) of synthetic monalidine A (**1**).
Page S18. Figure S13. ^{13}C NMR spectrum (100 MHz, DMSO- d_6) of synthetic monalidine A (**1**).
Page S19. Figure S14. ^1H NMR spectrum (600 MHz, DMSO- d_6) of arbusculidine A (**7**).
Page S20. Figure S15. ^{13}C NMR spectrum (150 MHz, DMSO- d_6) of arbusculidine (**7**).
Page S21. Figure S16. gHSQC spectrum (DMSO- d_6) of arbusculidine A (**7**).
Page S22. Figure S17. COSY spectrum (DMSO- d_6) of arbusculidine A (**7**).
Page S23. Figure S18. gHMBC spectrum (DMSO- d_6) of arbusculidine A (**7**).
Page S24. Figure S19. tROESY spectrum (DMSO- d_6) of arbusculidine A (**7**).
Page S25. Figure S20. $^{15}\text{NLRHMQC}$ spectrum (DMSO- d_6) of arbusculidine A (**7**).
Page S26. Figure S21. ^1H NMR spectrum (600 MHz, $\text{MeOH}-d_4$) of batzellamide A (**8**).
Page S27. Figure S22. ^{13}C NMR spectrum (150 MHz, $\text{MeOH}-d_4$) of batzellamide A (**8**).
Page S28. Figure S23. ^1H NMR spectrum (600 MHz, DMSO- d_6) of batzellamide A (**8**).
Page S29. Figure S24. ^{13}C NMR spectrum (150 MHz, DMSO- d_6) of batzellamide A (**8**).

- Page S30. Figure S25. gHSQC spectrum (DMSO-*d*₆) of batzellamide A (**8**).
Page S31. Figure S26. COSY spectrum (DMSO-*d*₆) of batzellamide A (**8**).
Page S32. Figure S27. gHMBC spectrum (DMSO-*d*₆) of batzellamide A (**8**).
Page S33. Figure S28. tROESY spectrum (DMSO-*d*₆) of batzellamide A (**8**).
Page S34. Figure S29. ¹⁵NHSQC spectrum (DMSO-*d*₆) of batzellamide A (**8**).
Page S35. Figure S30. ¹⁵NLRHMQC spectrum (DMSO-*d*₆) of batzellamide A (**8**).
Page S36. Figure S31. ¹H NMR spectrum (600 MHz, pyridine-*d*₅) of batzellamide A (**8**).
Page S37. Figure S32. ¹³C NMR spectrum (150 MHz, pyridine-*d*₅) of batzellamide A (**8**).
Page S38. Figure S33. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of hemibatzelladine J (**9**).
Page S39. Figure S34. ¹H NMR spectrum (150 MHz, DMSO-*d*₆) of hemibatzelladine J (**9**).
Page S40. Figure S35. gHSQC spectrum (DMSO-*d*₆) of hemibatzelladine J (**9**).
Page S41. Figure S36. COSY spectrum (DMSO-*d*₆) of hemibatzelladine J (**9**).
Page S42. Figure S37. gHMBC spectrum (DMSO-*d*₆) of hemibatzelladine J (**9**).
Page S43. Figure S38. tROESY spectrum (DMSO-*d*₆) of hemibatzelladine J (**9**).
Page S44. Figure S39. ¹⁵NHSQC spectrum (DMSO-*d*₆) of hemibatzelladine J (**9**).
Page S45. Figure S40. ¹⁵NLRHMQC spectrum (DMSO-*d*₆) of hemibatzelladine J (**9**).
Page S46. Figure S41. ¹H NMR spectrum (600 MHz, MeOH-*d*₄) of Δ¹⁹-hemibatzelladine J (**10**) and Δ²⁰-hemibatzelladine J (**11**).
Page S47. Figure S42. ¹³C NMR spectrum (150 MHz, MeOH-*d*₄) of Δ¹⁹-hemibatzelladine J (**10**) and Δ²⁰-hemibatzelladine J (**11**).
Page S48. Figure S43. gHSQC spectrum (MeOH-*d*₄) of Δ¹⁹-hemibatzelladine J (**10**) and Δ²⁰-hemibatzelladine J (**11**).
Page S49. Figure S44. COSY spectrum (MeOH-*d*₄) of Δ¹⁹-hemibatzelladine J (**10**) and Δ²⁰-hemibatzelladine J (**11**).
Page S50. Figure S45. gHMBC spectrum (MeOH-*d*₄) of Δ¹⁹-hemibatzelladine J (**10**) and Δ²⁰-hemibatzelladine J (**11**).
Page S51. Figure S46. tROESY spectrum (MeOH-*d*₄) of Δ¹⁹-hemibatzelladine J (**10**) and Δ²⁰-hemibatzelladine J (**11**).
Page S52. Figure S47. ¹H NMR spectrum (600 MHz, DMSO-*d*₄) of Δ¹⁹-hemibatzelladine J (**10**) and Δ²⁰-hemibatzelladine J (**11**).
Page S53. Figure S48. ¹³C NMR spectrum (150 MHz, DMSO-*d*₄) of Δ¹⁹-hemibatzelladine J (**10**) and Δ²⁰-hemibatzelladine J (**11**).

Table S1. NMR Data (^1H 600 MHz, ^{13}C 150 MHz, ^{15}N , pyridine- d_5) for Batzellamide A (**8**).

Position	8^a	8^b
1	20.4	1.17, d (6.2)
2	46.2	3.30, m
3	36.0	1.41, m; 1.39, m
4	56.3	3.34, m
5	30.5	1.90, m
6	30.5	1.90, m
7	56.3	3.34, m
8	35.0	1.79, m; 1.45, m
9	50.8	3.21, m
10	150.5	
11	34.0	1.94, m; 1.00, ddd (1.5, 11.4, 22.8)
12	30.0	1.24, m
13	29.6	1.24, m
14	29.8	1.24, m
15	29.7	1.24, m
16	25.9/25.8	1.24, m
17	36.2/36.1	1.58, m; 1.42, m
18	73.0	5.00, m
19	20.3	1.22, d (6.4)
20	169.2	
21	43.8/43.6	3.23, m
22	57.3/57.0	4.03, m
23	28.8	2.28, m
24	30.8	2.14, m; 1.61, m
25	56.2/56.1	3.90, m
26	38.1	2.93, bd (16.3); 2.58, bdd (14.8, 14.5)
27	169.1	
28	151.0	
29	50.1/50.0	4.00, m
30	17.5	1.49, d (6.7)
N-H		10.08, s
N-H		9.79, s

^a150 MHz; ^b600 MHz

Table S2. NMR Data (¹H 600 MHz, ¹³C 150 MHz, ¹⁵N, DMSO-*d*₆) for Batzellamide A (**8**).

Position	8^a	8^b
1	19.8*	1.17, d (6.2)*
2	45.3	3.45, m
3	34.0	1.45, m; 1.32, m
4	55.6	3.65, m
5	29.5	2.10, m; 1.57, m
6	29.5	2.10, m; 1.57, m
7	55.5	3.65, m
8	32.9	2.16, m; 1.15, m
9	49.5	3.32, m
N-9a	-296	
10	149.2	
N-10a	-293	
11	28.7	1.24, m
12	24.5	1.24, m
13	28.6	1.24, m
14	29.5	1.24, m
15	29.6	1.24, m
16	24.7	1.24, m
17	34.9	2.15, m; 1.17, m
18	71.6	4.86, tq (6.3, 7.0)
19	19.8*	1.17, d (6.3)*
20	168.5 [#]	
21	43.0/42.6	3.20, dd (8.0, 3.6)
22	55.9	4.06, m
23	27.5	2.27, ddd (12.3, 6.1, 6.0); 1.45 (m)
24	29.6	2.18, m; 1.67, m
25	54.8/54.7	3.75, m
26	36.8	2.81, dd (16.4, 3.8); 2.74, bdd (16.3, 13.5)
27	168.4 [#]	
N-27a	-243	11.88, bs
28	148.5	
N-28a	-282	11.99, bs
29	48.5/48.4	3.93, m
30	16.8	1.22, d (6.4)
N-H		10.08, s
N-H		9.79, s

^a150 MHz; ^b600 MHz; ^{*,#} assignments may be interchanged.

Table S3. NMR Data (¹H 600 MHz, ¹³C 150 MHz, ¹⁵N, DMSO-*d*₆) for Hemibatzelladines Δ¹⁹ (**10**) and Δ²⁰ (**11**).

Position	10 ^a	10 ^b	11 ^a	11 ^b
1	156.6	-	156.6	-
2	40.2	3.11, dd (13.1; 6.7)	40.2	3.11, dd (13.1; 6.7)
3	25.4	1.61, m	25.4	1.61, m
4	25.2	1.51, m	25.2	1.51, m
5	63.5	4.10, m	63.5	4.10, m
6	164.3	-	164.3	-
7	100.4	-	100.4	-
8	148.3	-	148.3	-
9	30.0	2.76, m; 3.16, ddd (18.1, 8.7, 8.2)	30.0	2.76, m; 3.16, ddd (18.1, 8.7, 8.2)
10	28.7	2.23, m; 16.2, m	28.7	2.23, m; 16.2, m
11	56.6	3.83, m	56.6	3.83, m
12	31.0	3.16, dbr (14.4); 1.44, m	31.0	3.16, dbr (14.4); 1.44, m
13	51.1	3.53, m	51.1	3.53, m
14	147.2	-	147.2	-
15	46.5	4.42, q (6.0)	46.5	4.42, q (6.0)
16	24.0	1.26, d (6.0)	24.0	1.27, d (6.0)
17	25.9	1.50, m	25.9	1.50, m
18	35.4	1.76, m	23.7	2.20, m
19	131.8	5.47, m	35.8	1.66, m
20	127.8	5.45, m	131.7	5.47, m
21	24.6	2.18, m	129.3	5.41, m
22	33.4	1.58, m	31.7	2.27, bq (7.2)
23	62.5	3.55, t (6.1)	62.5	3.54, t (6.1)
NH-1a	-295	7.53, t (5.2)	-295	7.53, t (5.2)
NH-13a	-285	8.78, bs	-285	8.72, bs
NH-14a	-290	8.43, bs	-290	8.32, bs

^a150 MHz; ^b600 MHz. ¹⁵N assignments were not calibrated with an external standard. The δ value has an accuracy of about 1 ppm in reference to CH₃NO₂ (0 ppm) and are assigned based on ¹⁵NHSQC and ¹⁵NlrHMQC correlations.

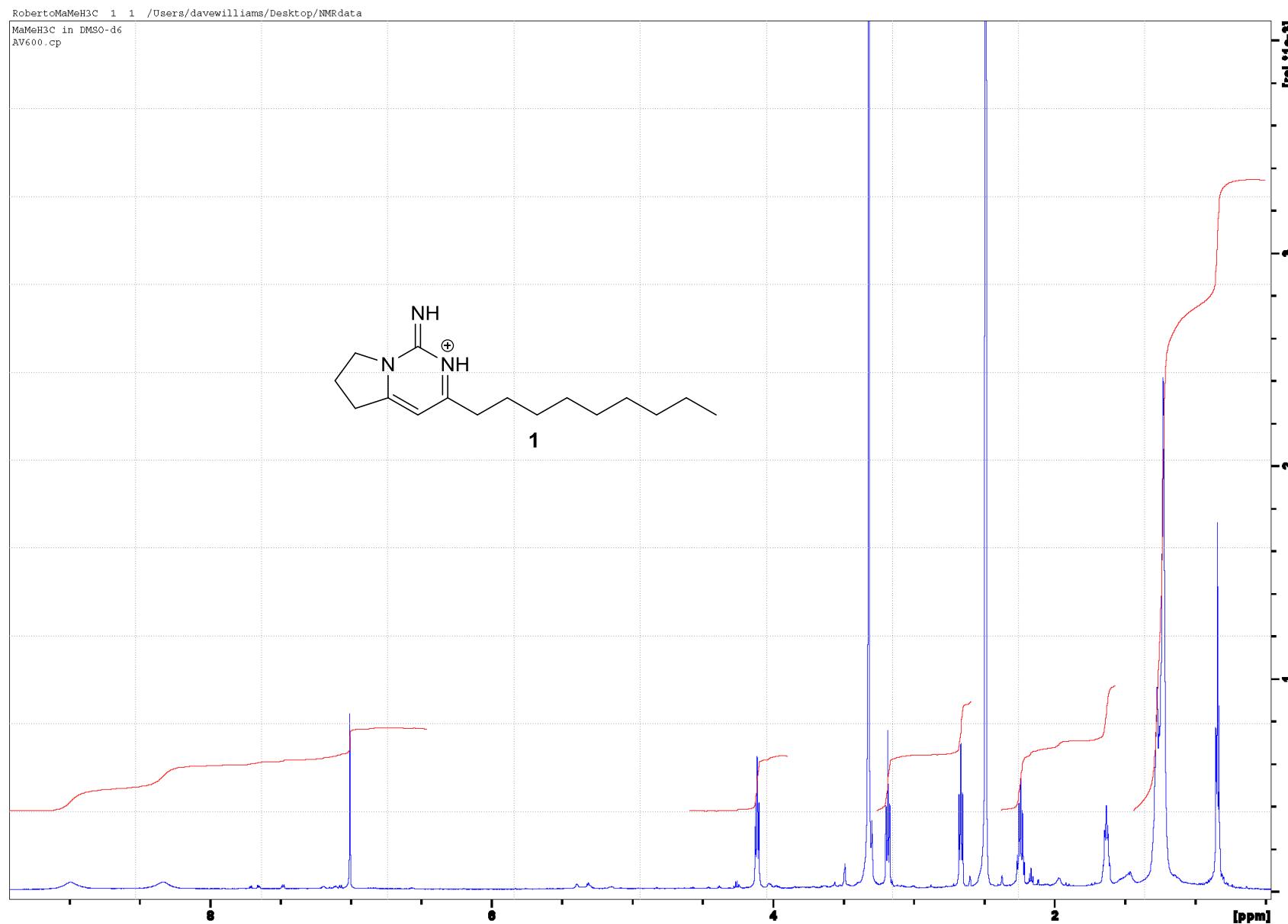


Figure S1. ¹H NMR spectrum (600 MHz, DMSO-d₆) of monalidine A (**1**).

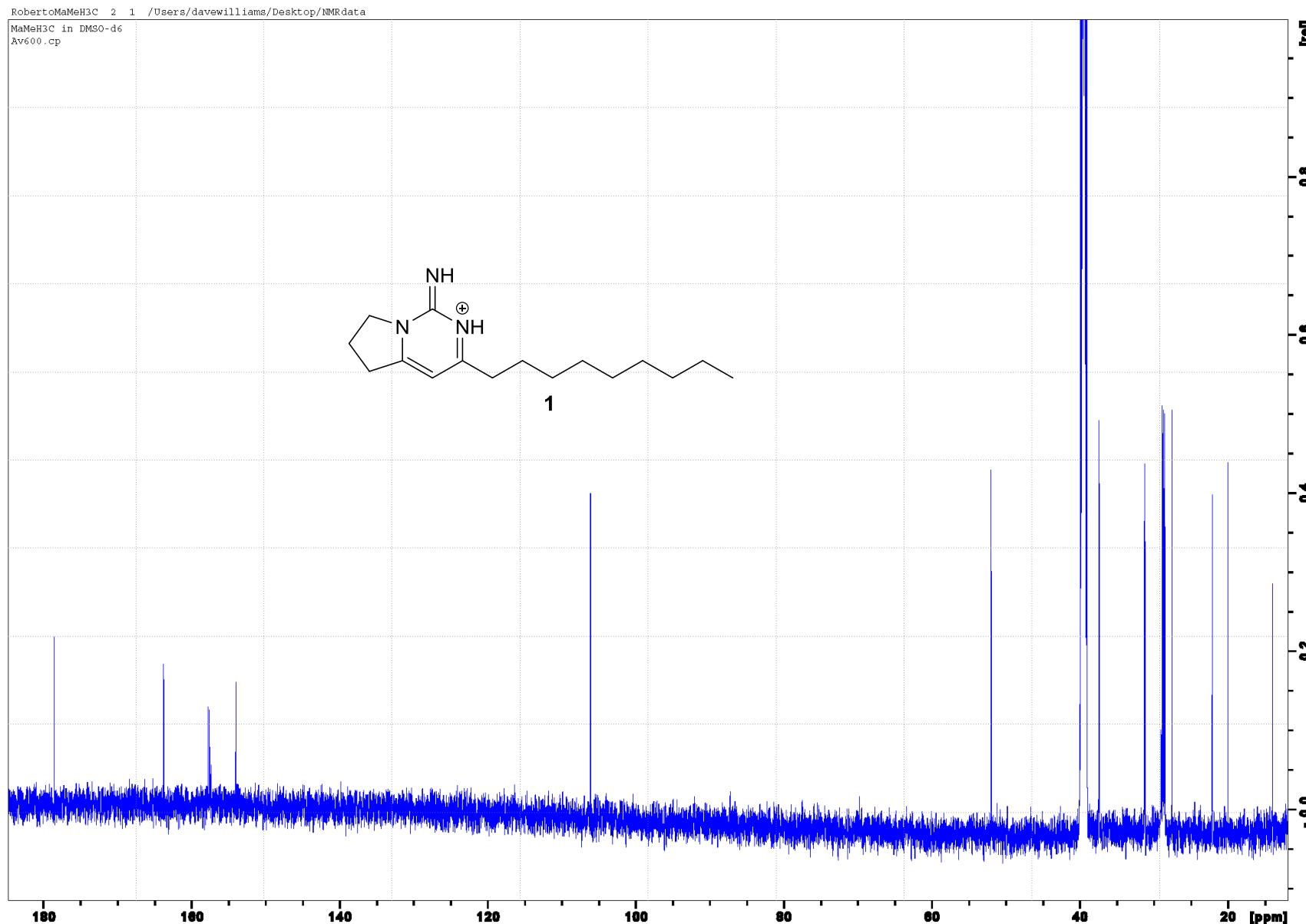


Figure S2. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of monalidine A (**1**).

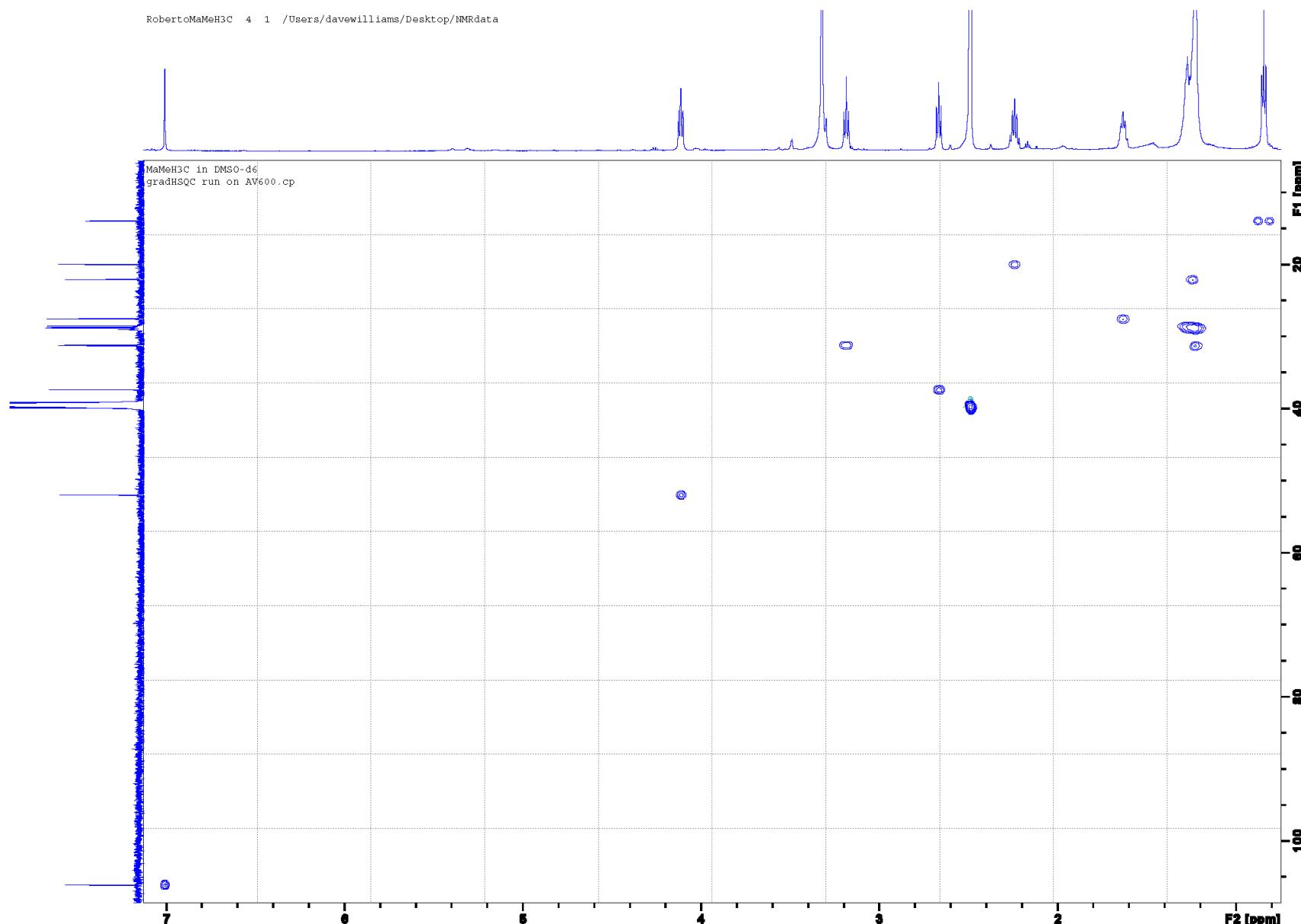


Figure S3. gHSQC spectrum (DMSO-*d*₆) of monalidine A (**1**).

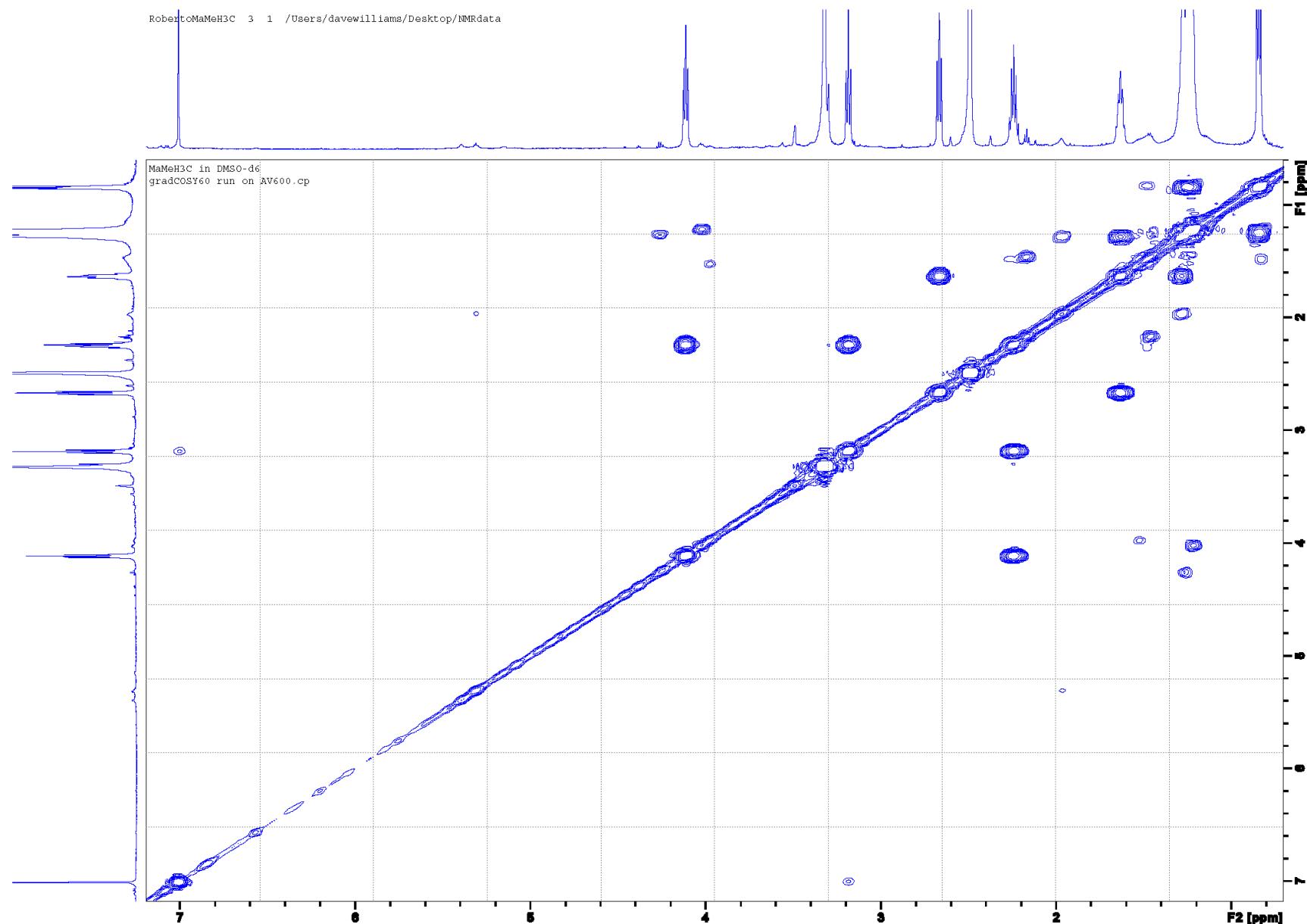


Figure S4. COSY spectrum (DMSO-*d*₆) of monalidine A (**1**).

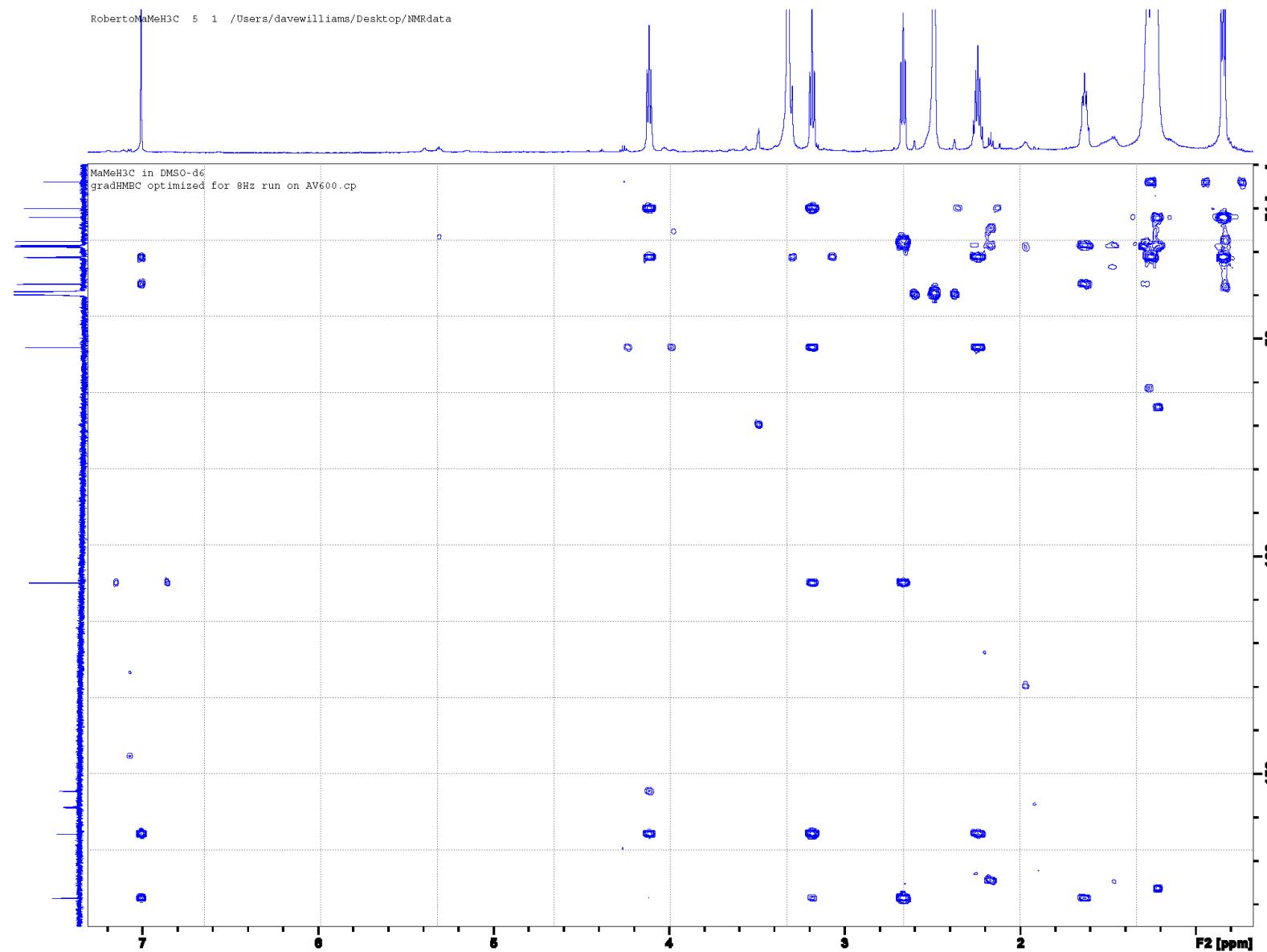


Figure S5. gHMBC spectrum (DMSO-*d*₆) of monalidine A (**1**).

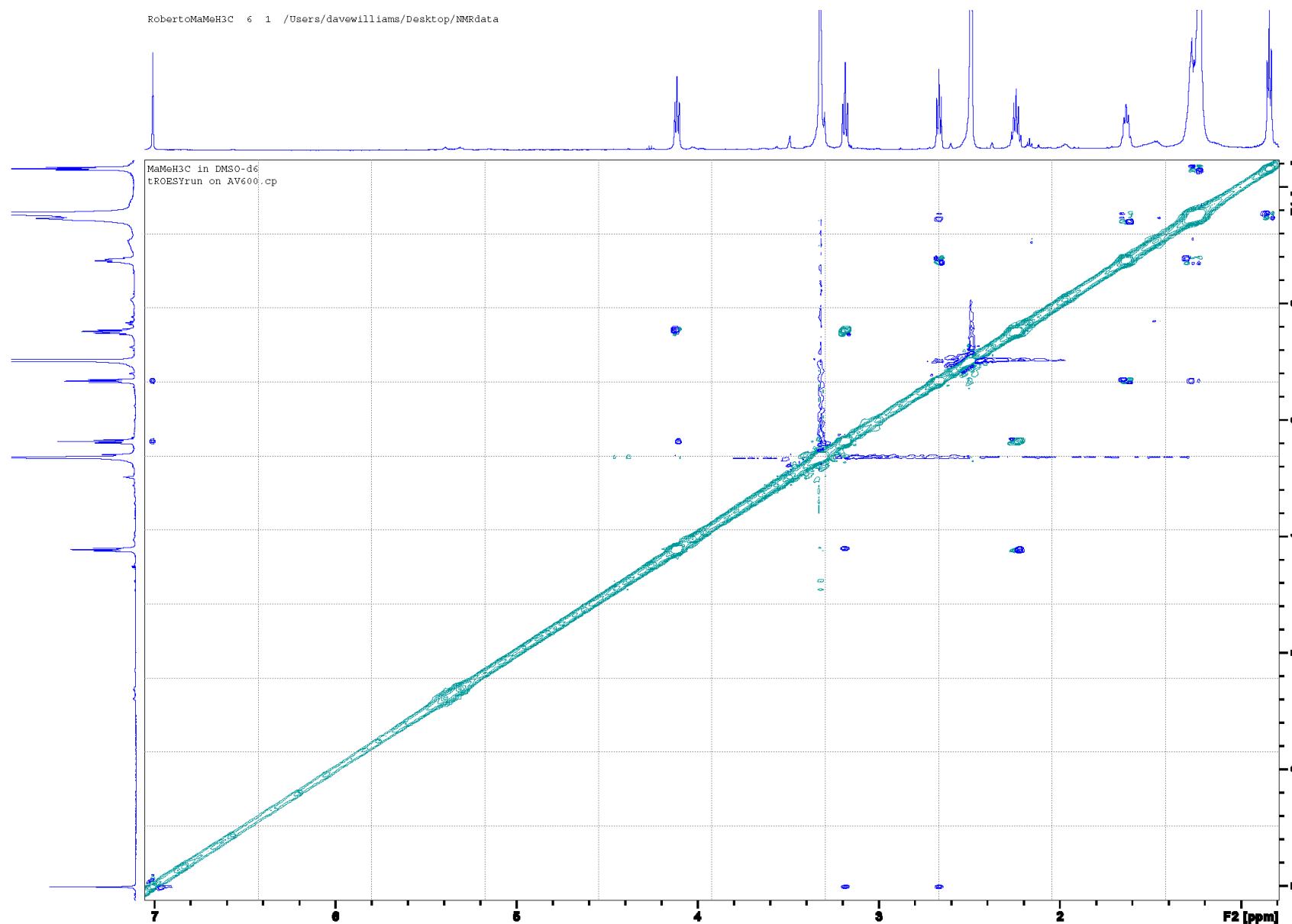


Figure S6. tROESY spectrum (DMSO-*d*₆) of monalidine A (**1**).

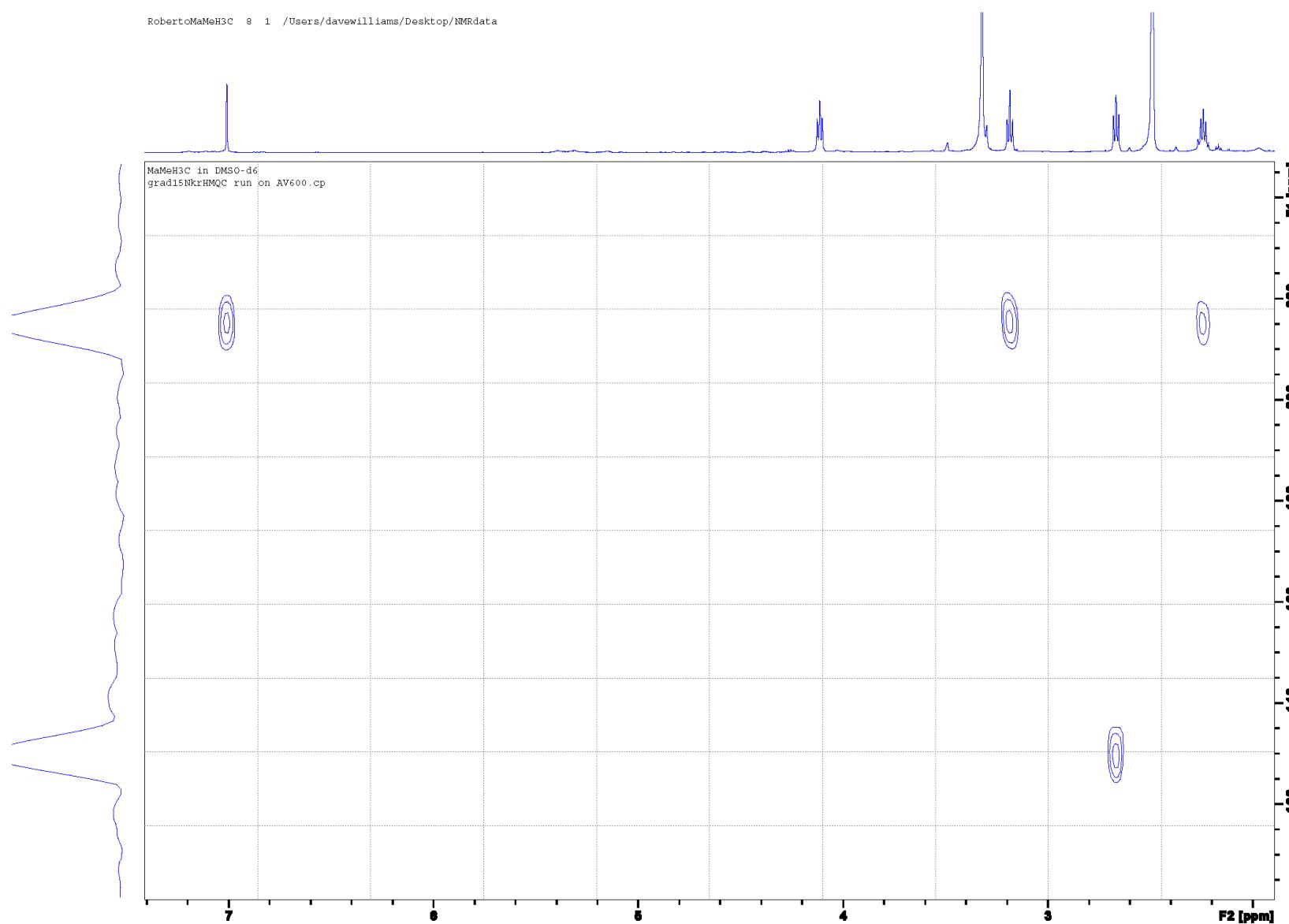
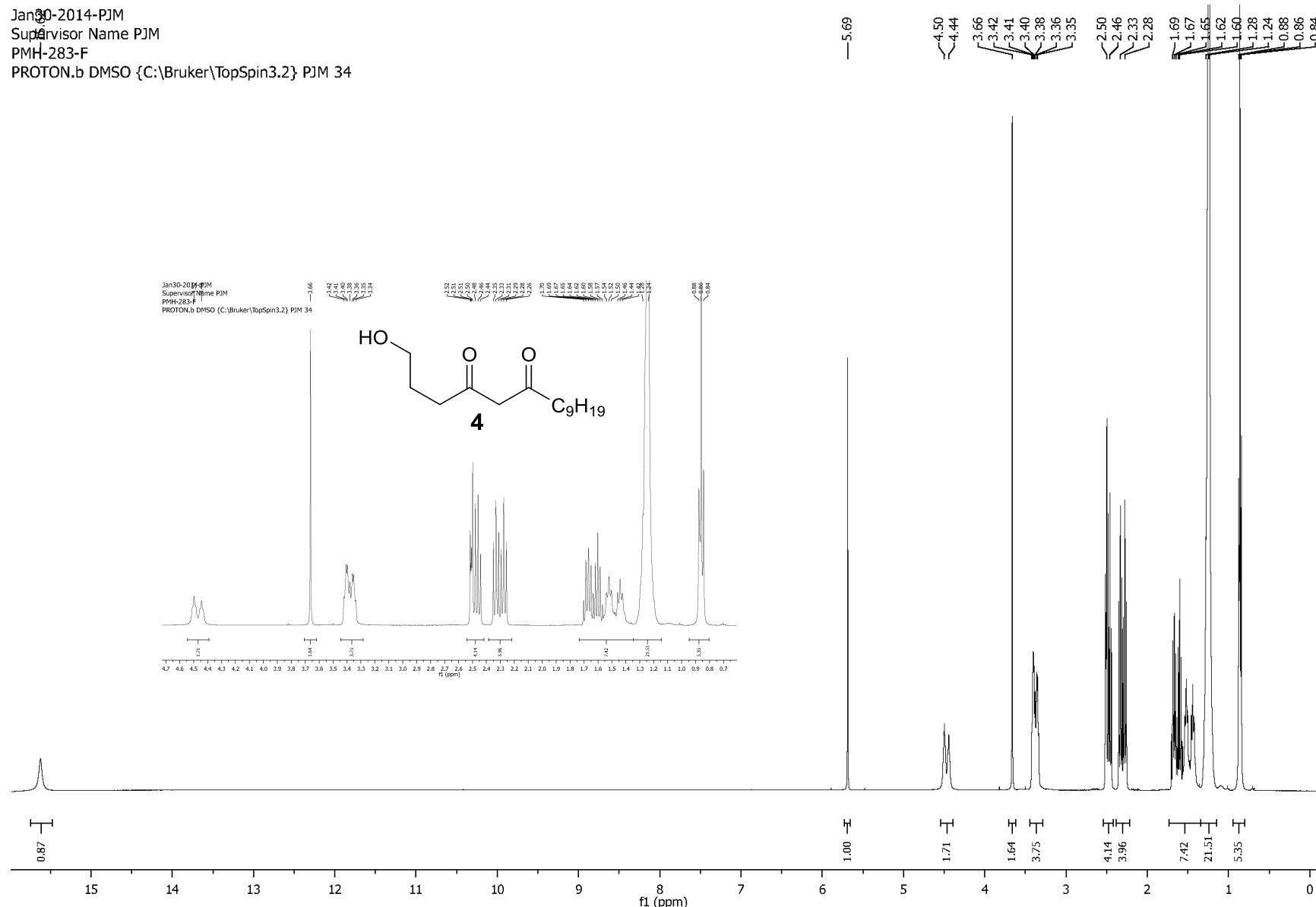


Figure S7. ¹⁵NLRHMQC spectrum (DMSO-*d*₆) of monalidine A (**1**).

Jan30-2014-PJM
 Supervisor Name PJM
 PMH-283-F
 PROTON.b DMSO {C:\Bruker\TopSpin3.2} PJM 34



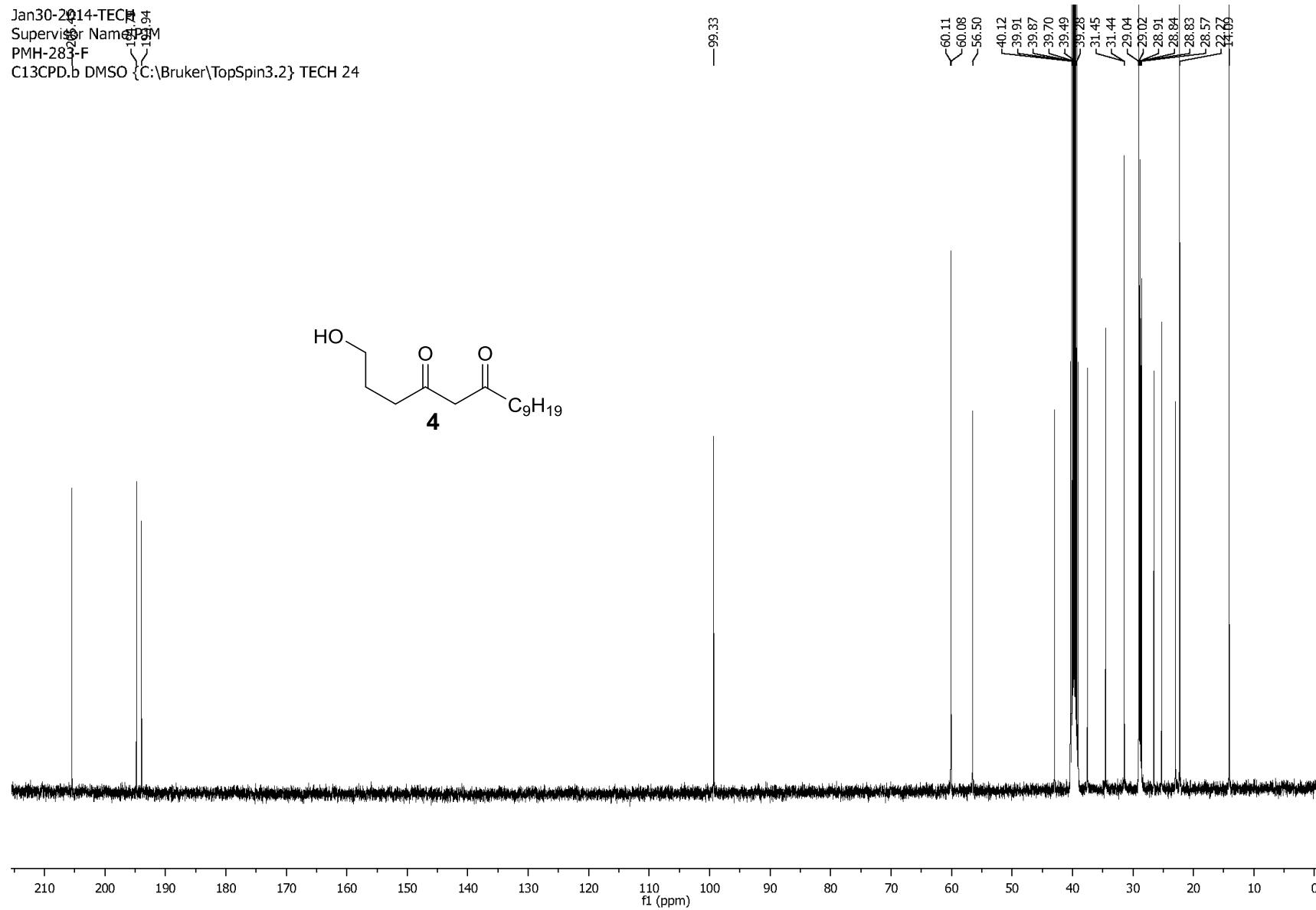


Figure S9. ¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of 1-hydroxypentadecane-4,6-dione (**4**).

Jan20-2014-PJM
Supervisor Name PJM
PMH-280-3
PROTON.b CDCl₃ {C:\Bruker\TopSpin3.2} PJM 25

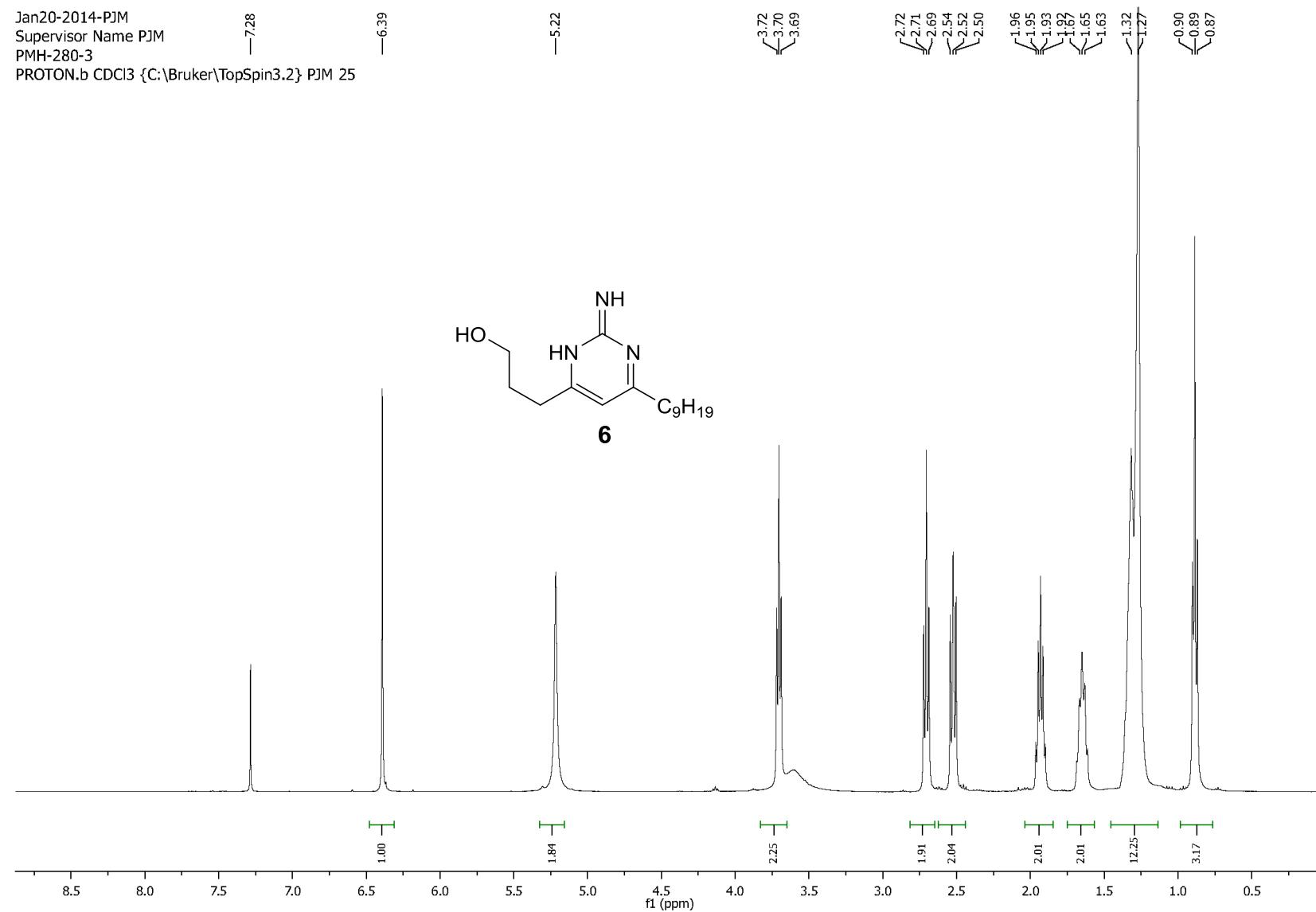


Figure S10. ¹H NMR spectrum (400 MHz, CDCl₃) of 3-(2-imino-6-nonyl-2,3-dihydropyrimidin-4-yl)propan-1-ol (**6**).

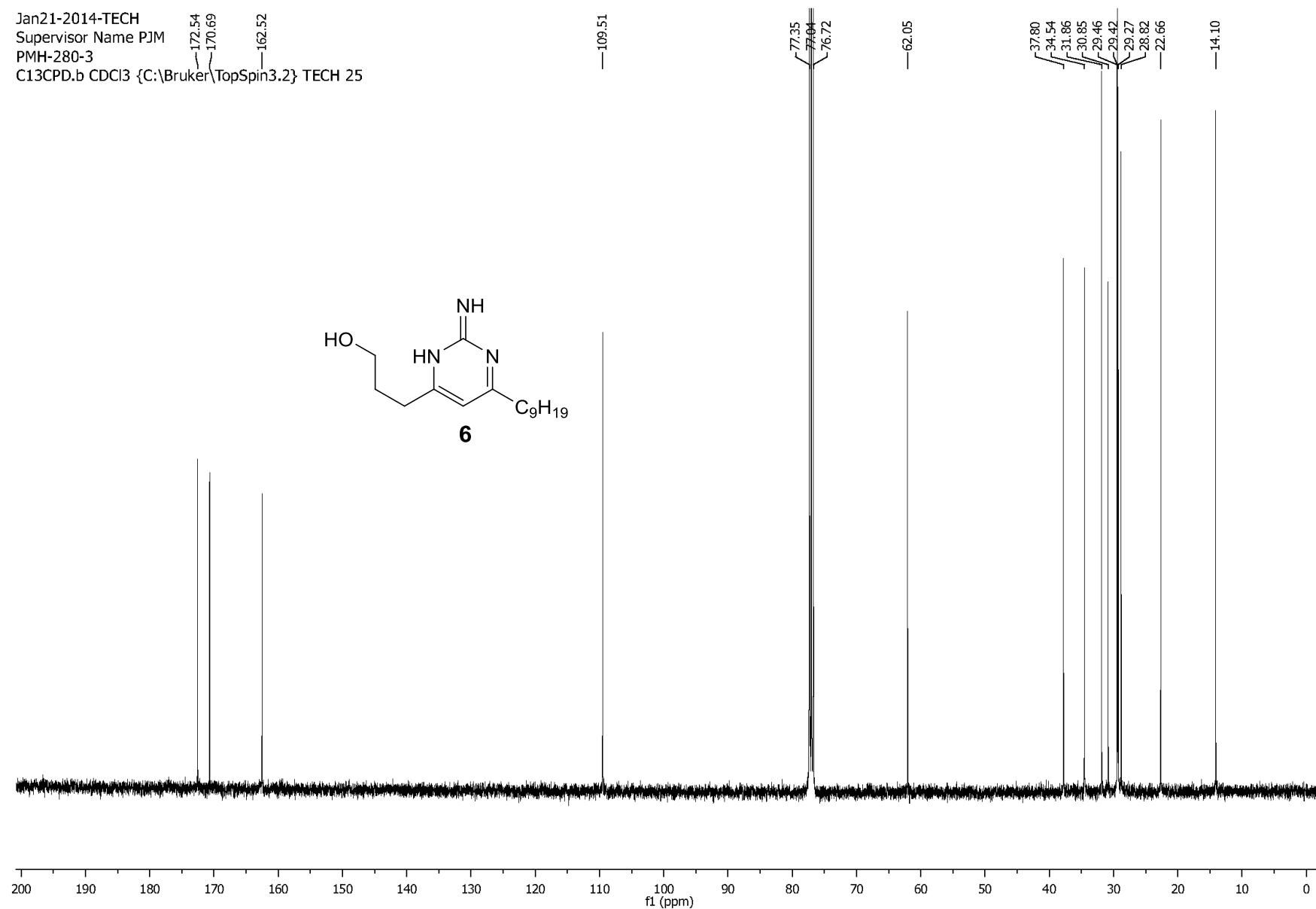


Figure S11. ¹³C NMR spectrum (100 MHz, CDCl₃) of 3-(2-imino-6-nonyl-2,3-dihydropyrimidin-4-yl)propan-1-ol (**6**).

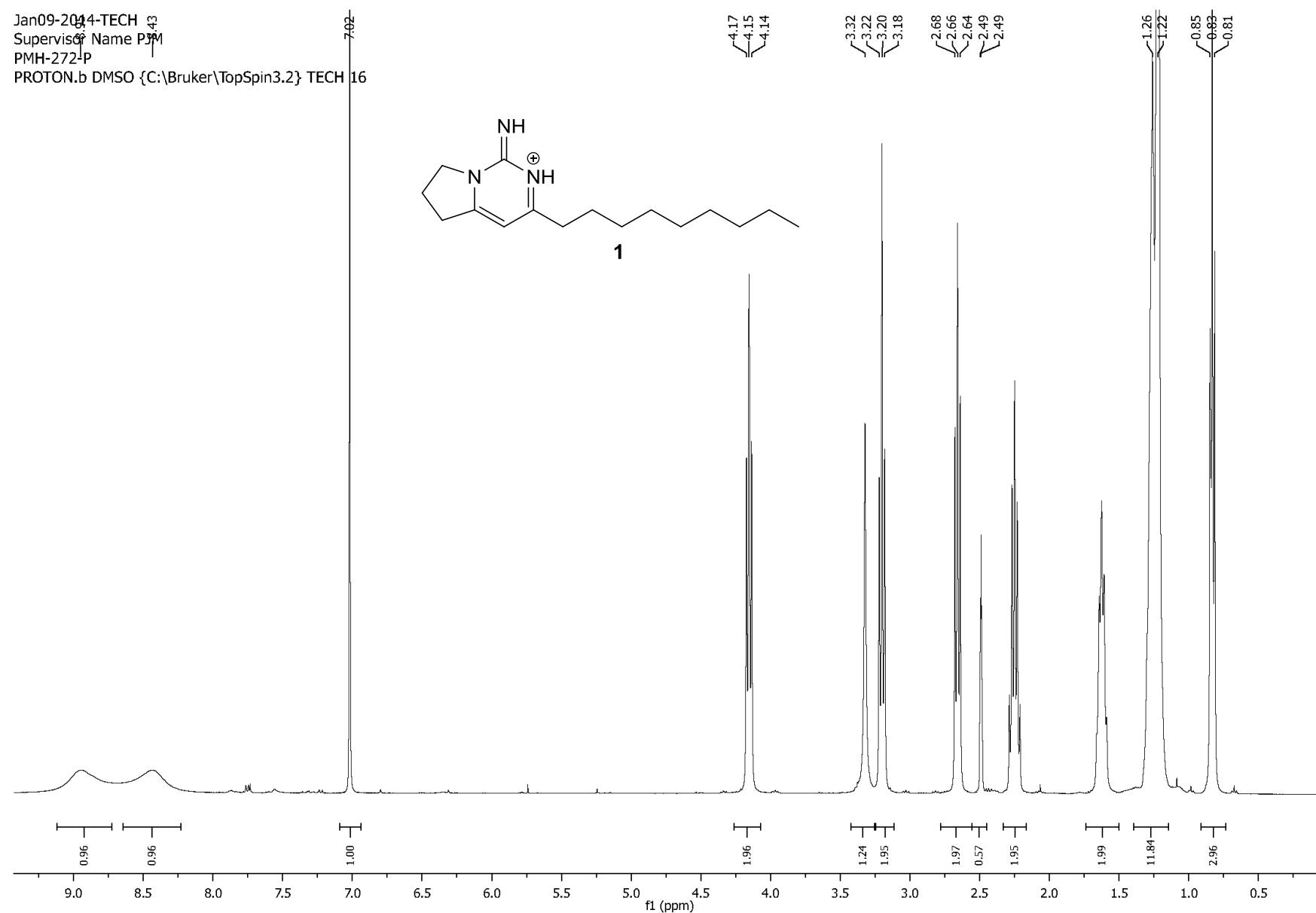


Figure S12. ^1H NMR spectrum (400 MHz, DMSO- d_6) of synthetic monalidine A (1).

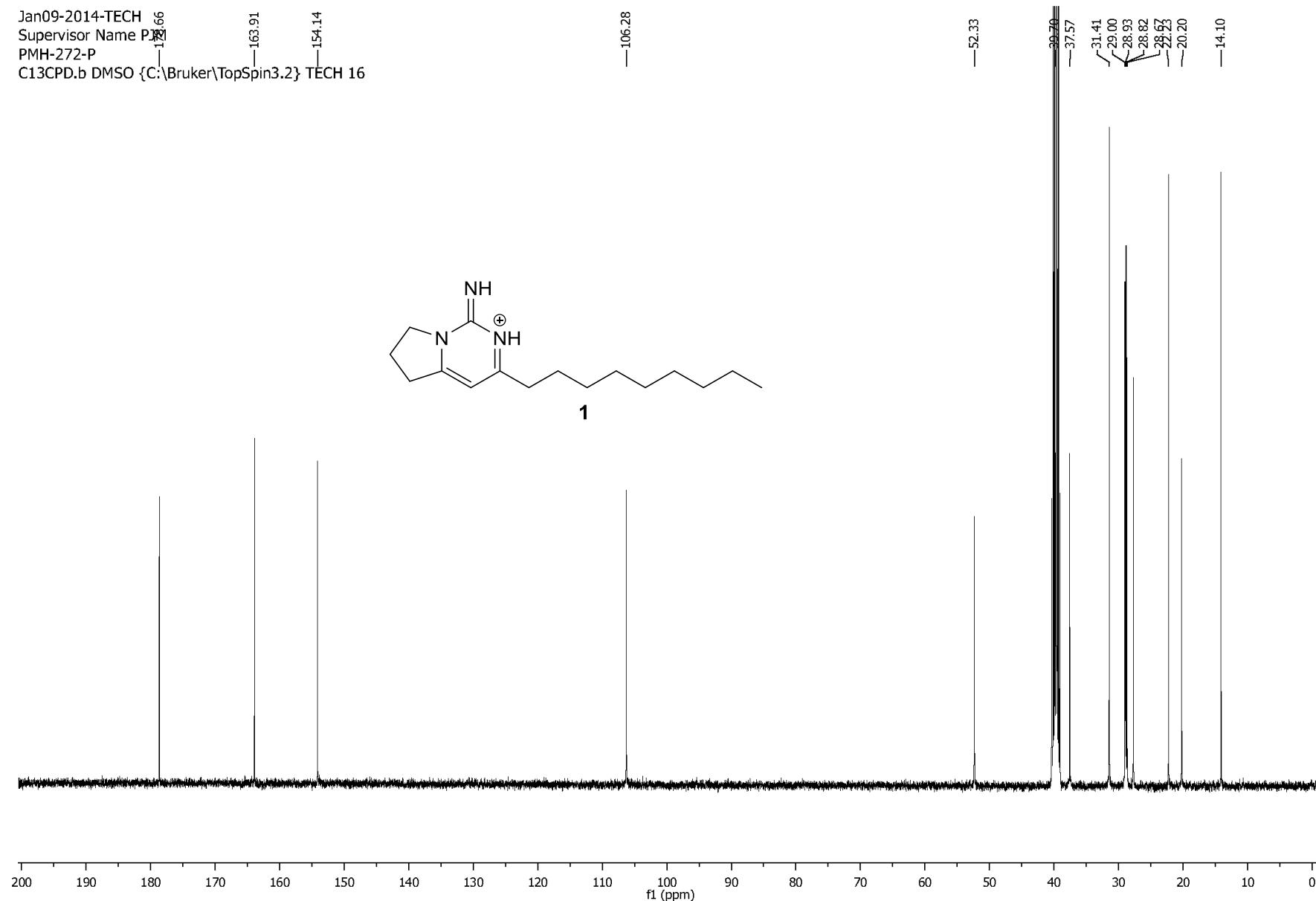


Figure S13. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of synthetic monalidine A (**1**).

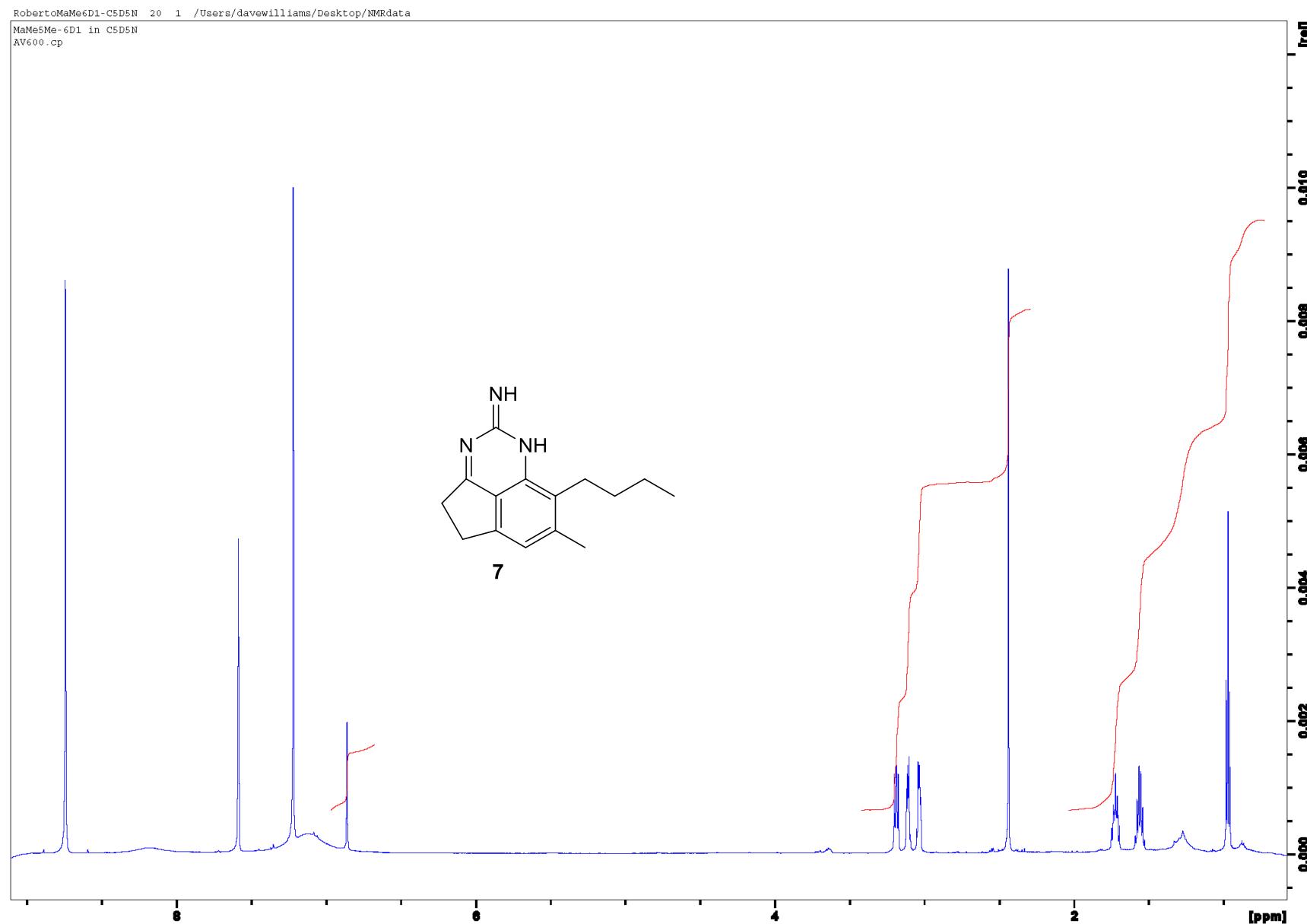


Figure S14. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of arbusculidine A (**7**).

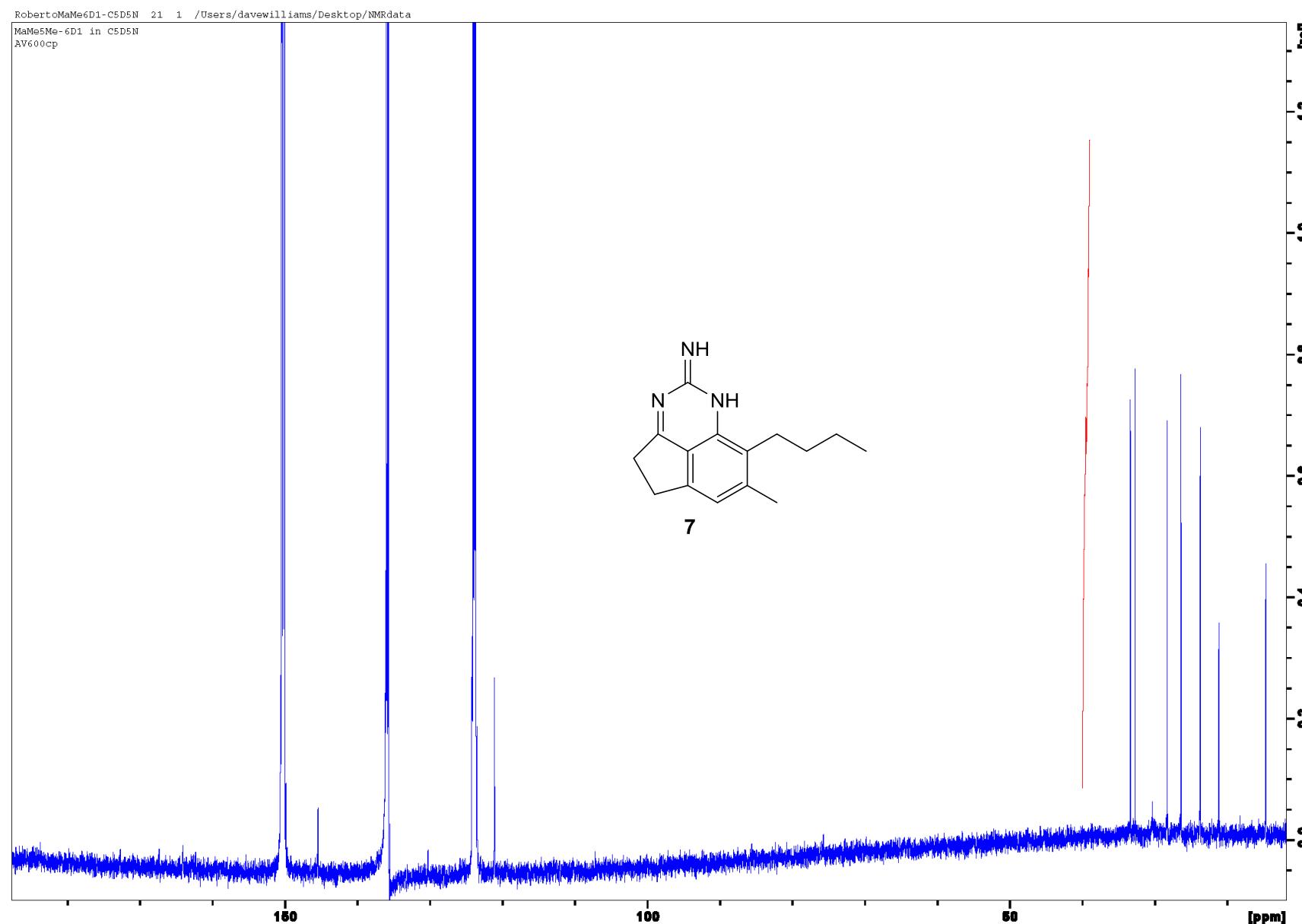


Figure S15. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of arbusculidine A (**7**).

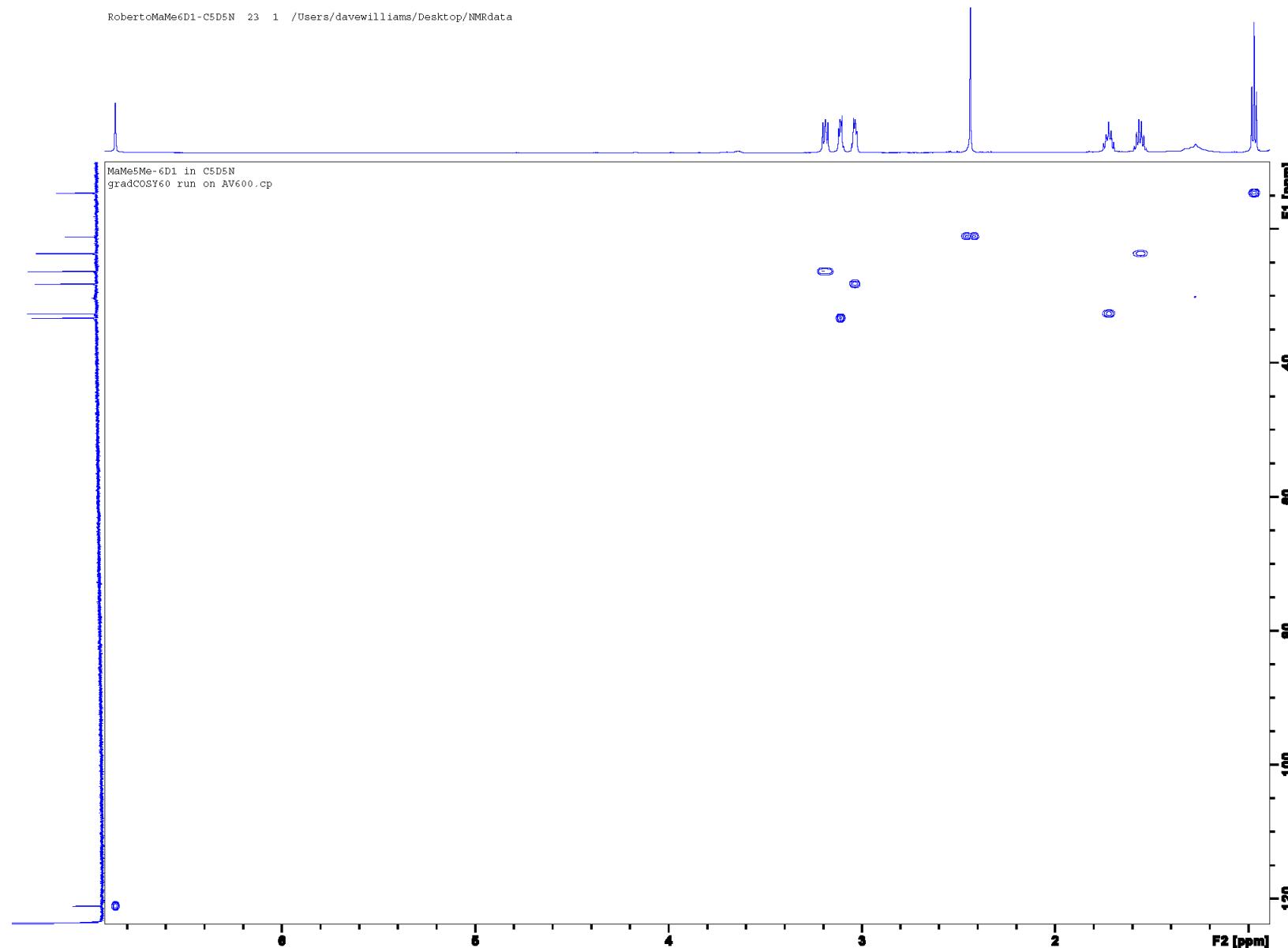


Figure S16. gHSQC spectrum ($\text{DMSO}-d_6$) of arbusculidine A (7).

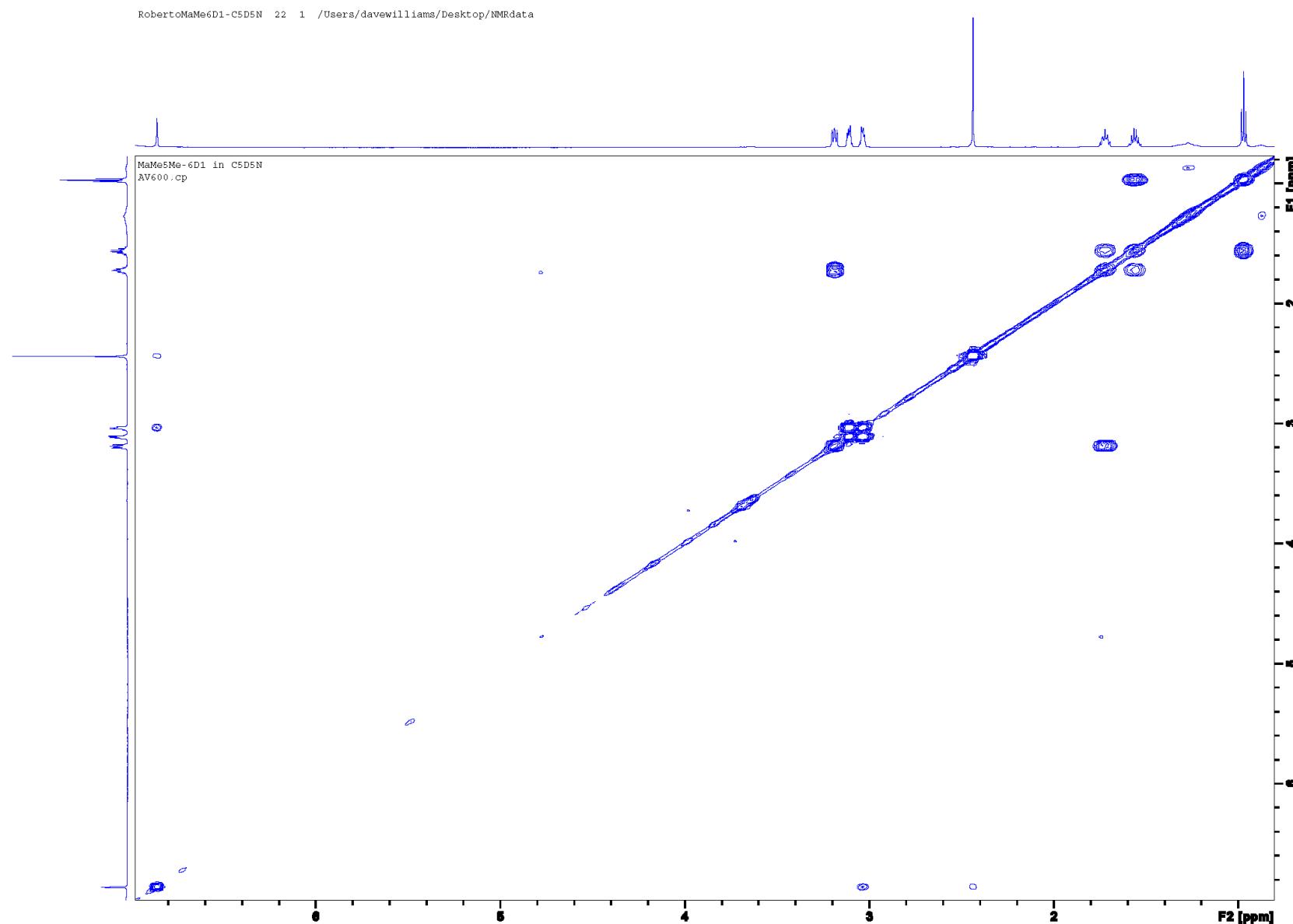


Figure S17. COSY spectrum ($\text{DMSO}-d_6$) of arbusculidine A (7).

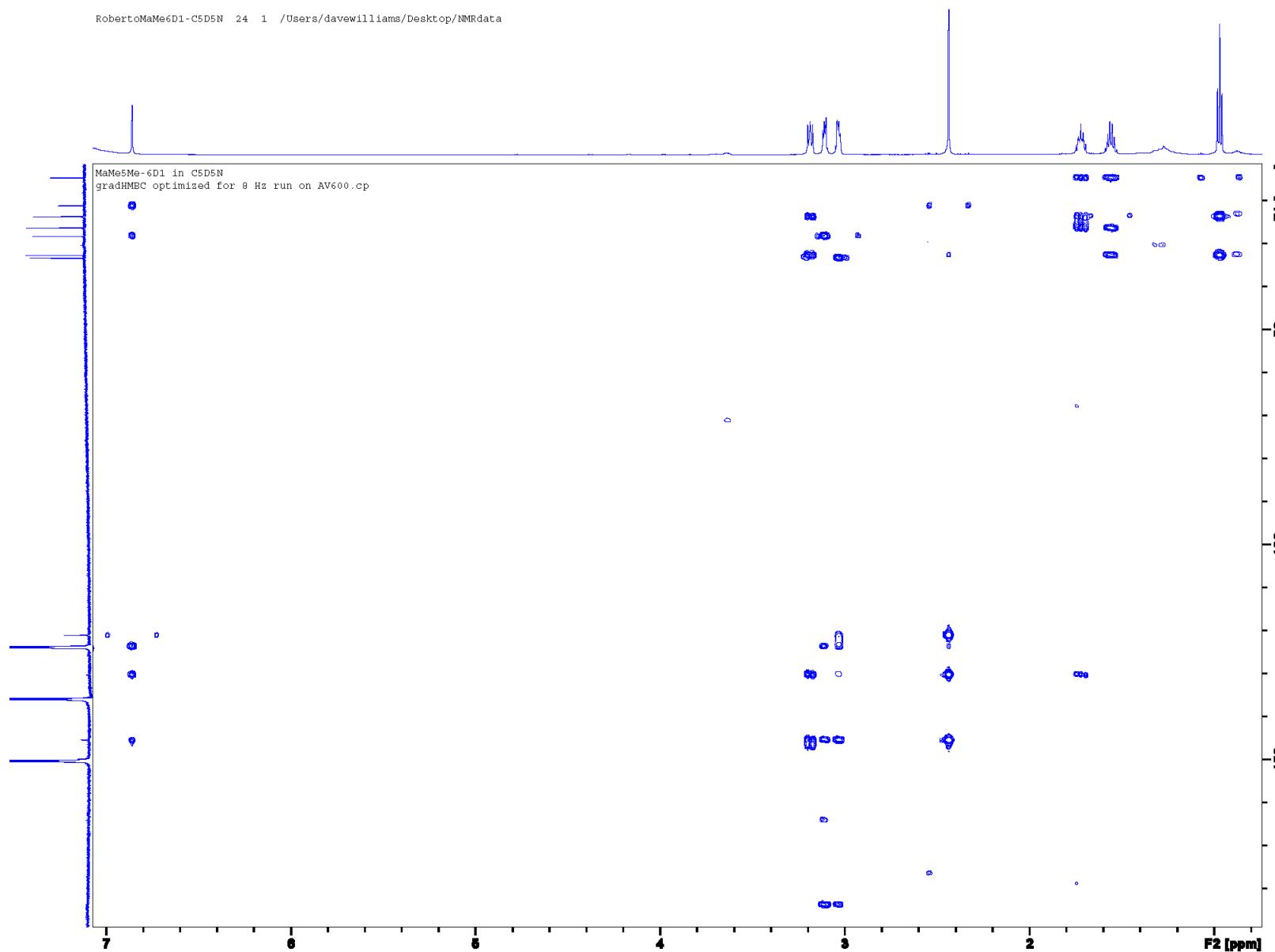


Figure S18. gHMBC spectrum ($\text{DMSO}-d_6$) of arbusculidine A (7).

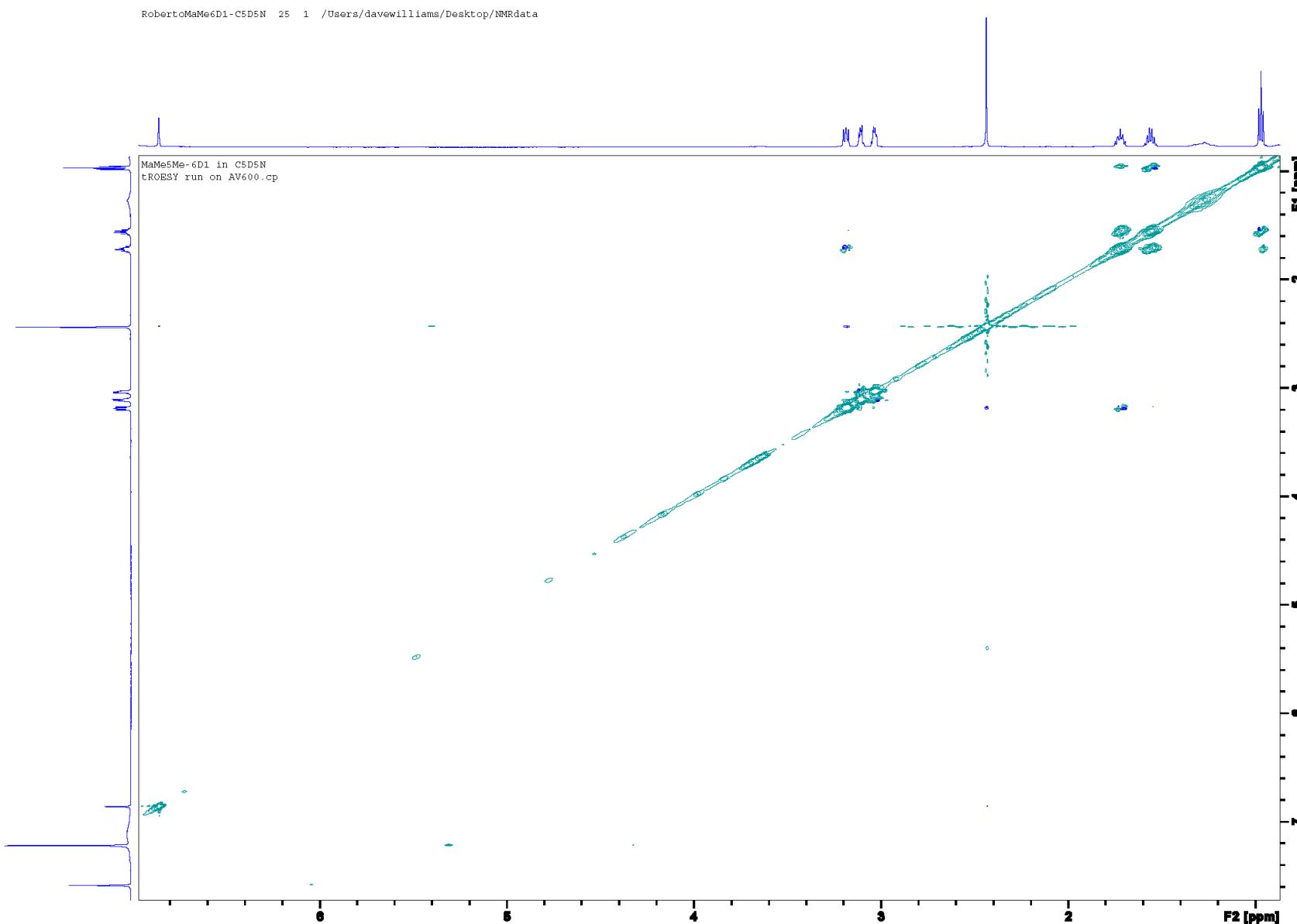


Figure S19. tROESY spectrum (DMSO-*d*₆) of arbusculidine A (**7**).

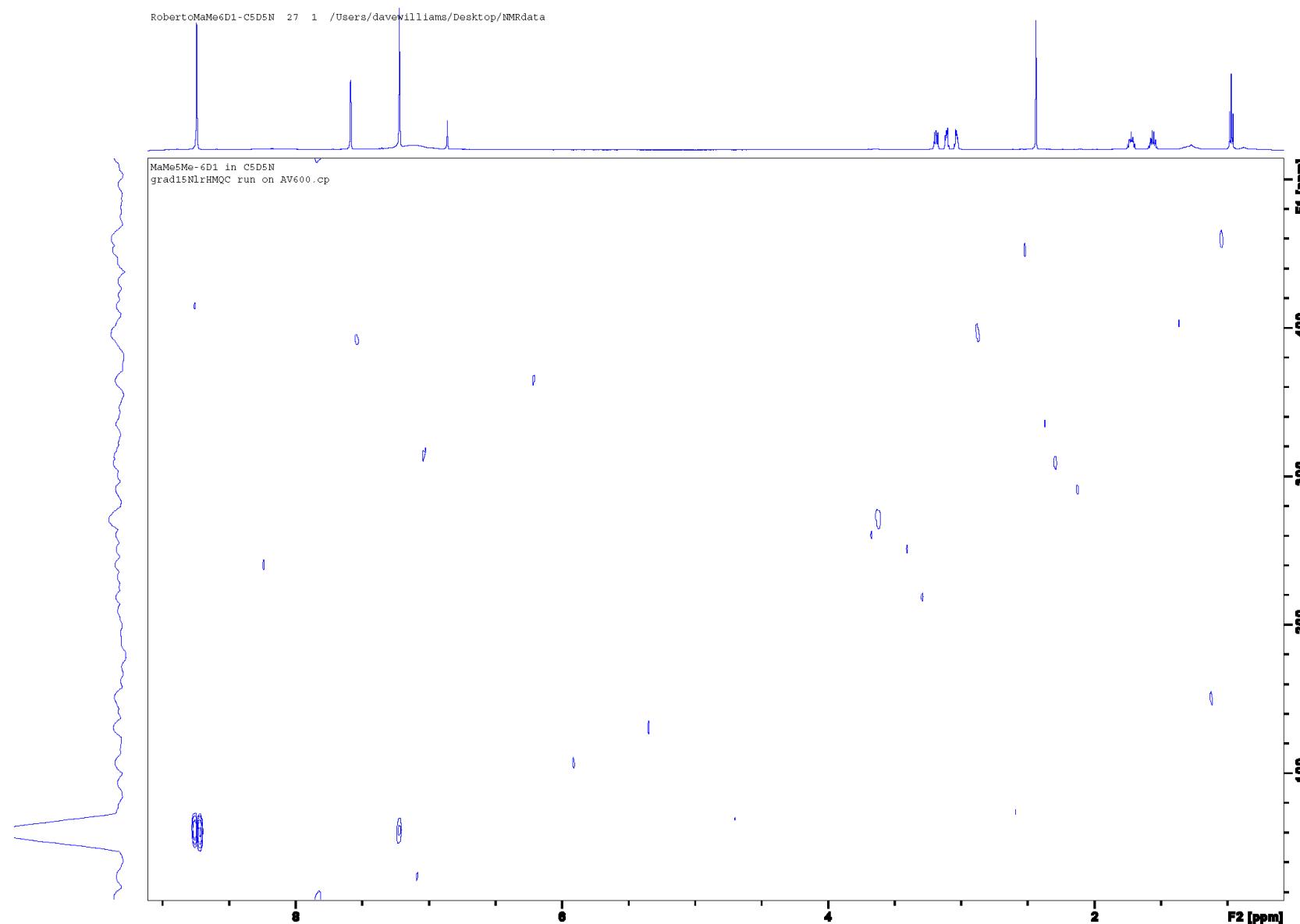


Figure S20. ^{15}N LRRHMQC spectrum ($\text{DMSO}-d_6$) of arbusculidine A (7).

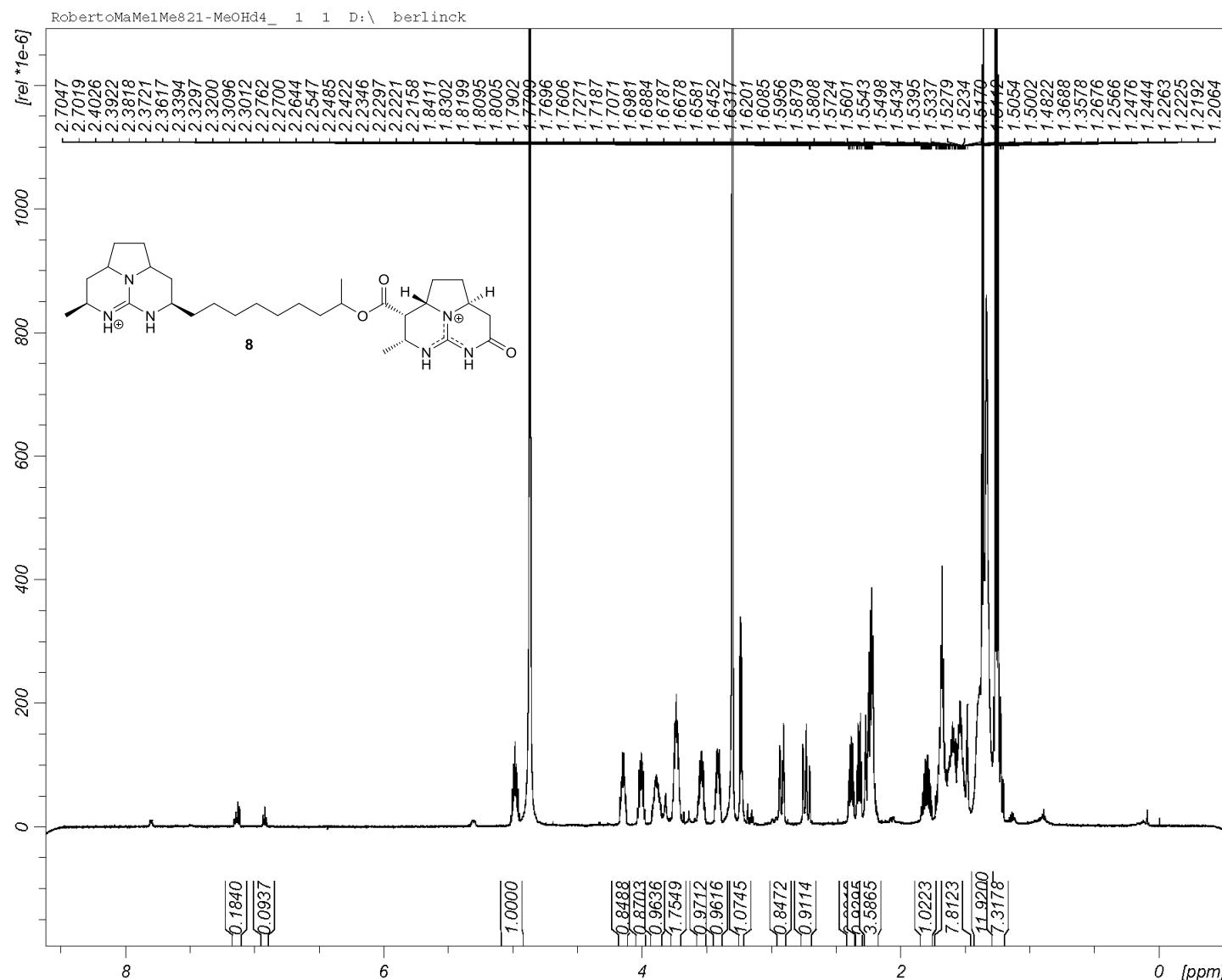


Figure S21. ^1H NMR spectrum (600 MHz, $\text{MeOH}-d_4$) of batzellamide A (**8**).

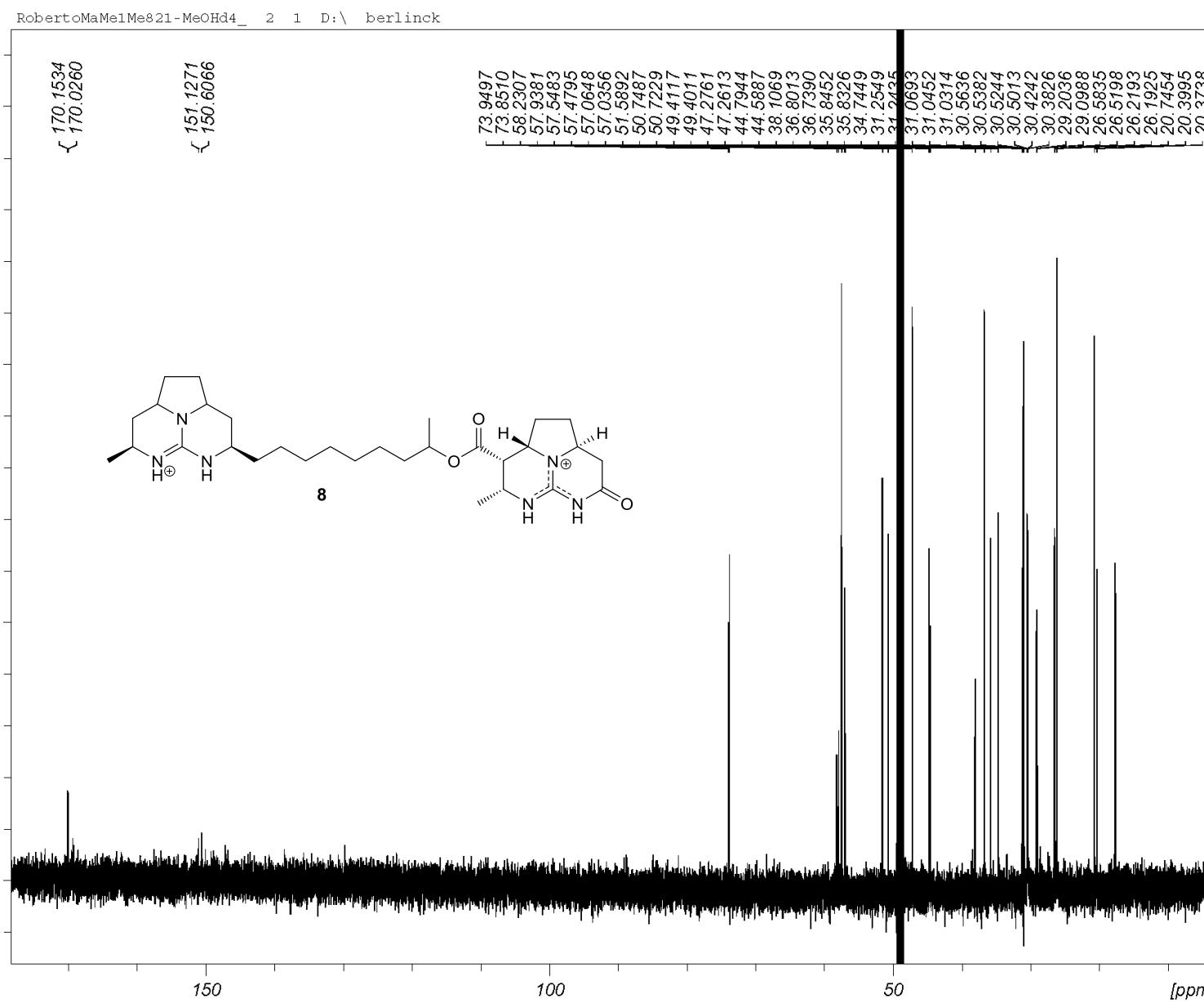


Figure S22. ¹³C NMR spectrum (150 MHz, MeOH-*d*₄) of batzellamide A (**8**).

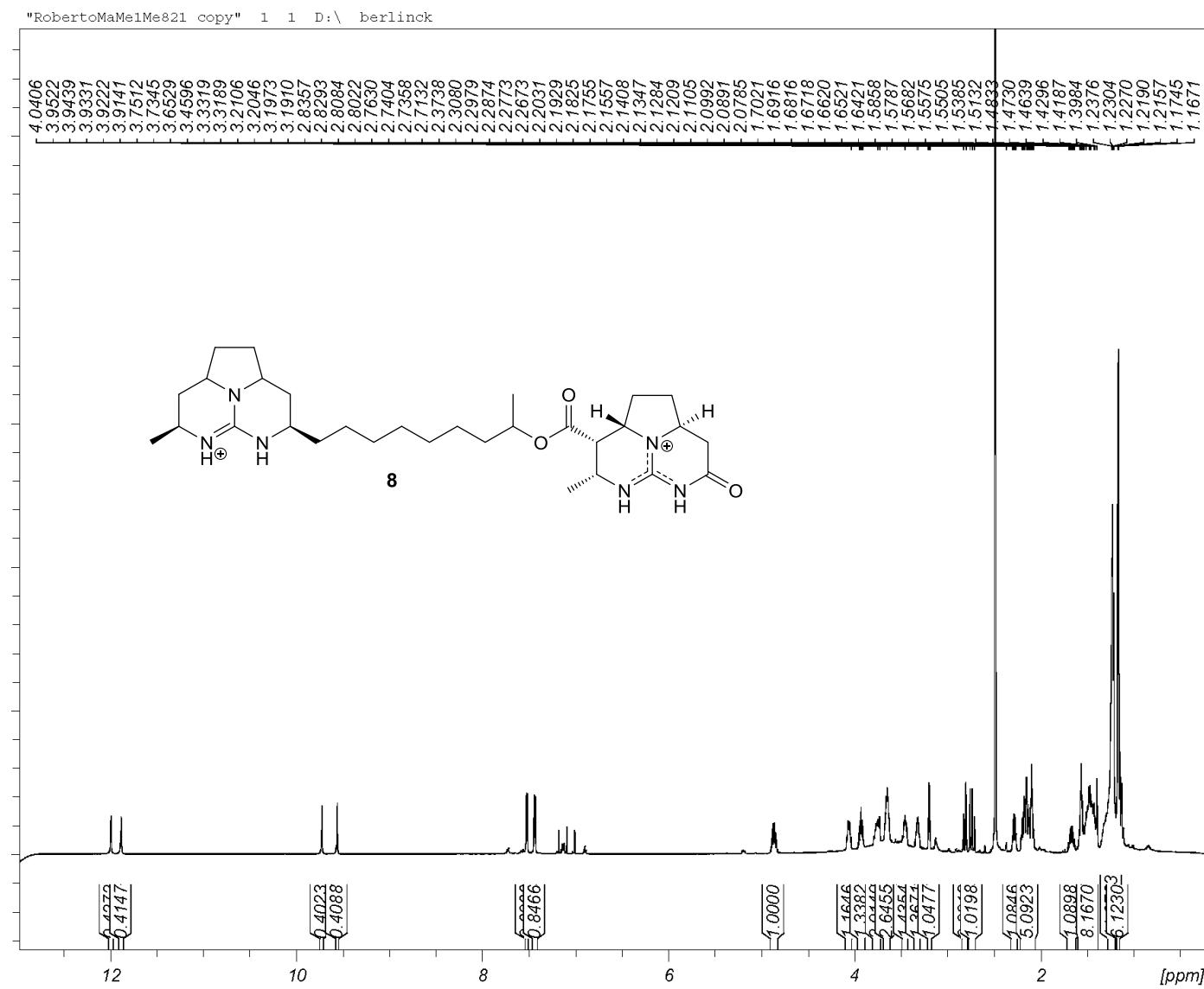


Figure S23. ^1H NMR spectrum (600 MHz, DMSO- d_6) of batzellamide A (**8**).

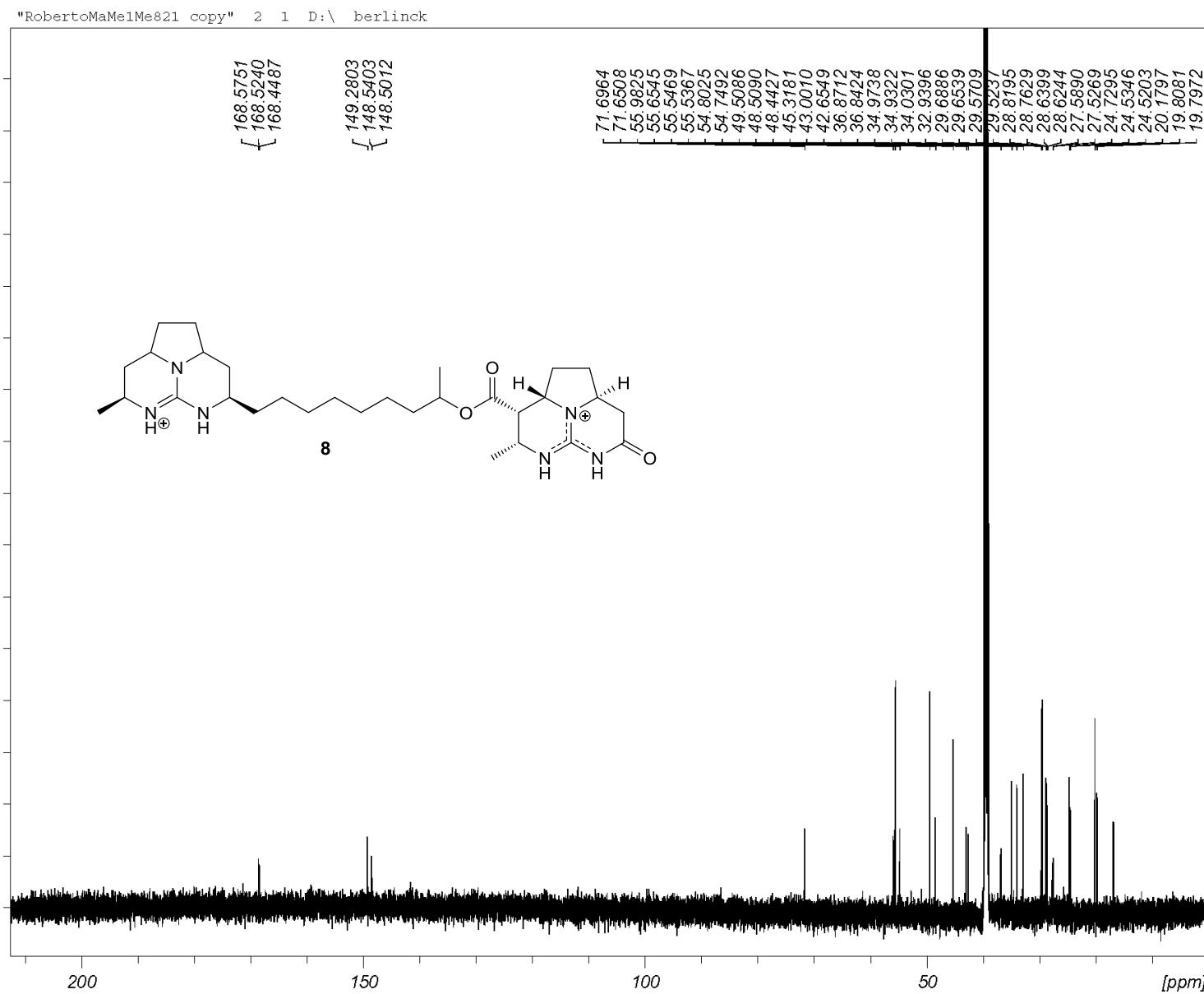


Figure S24. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of batzellamide A (**8**).

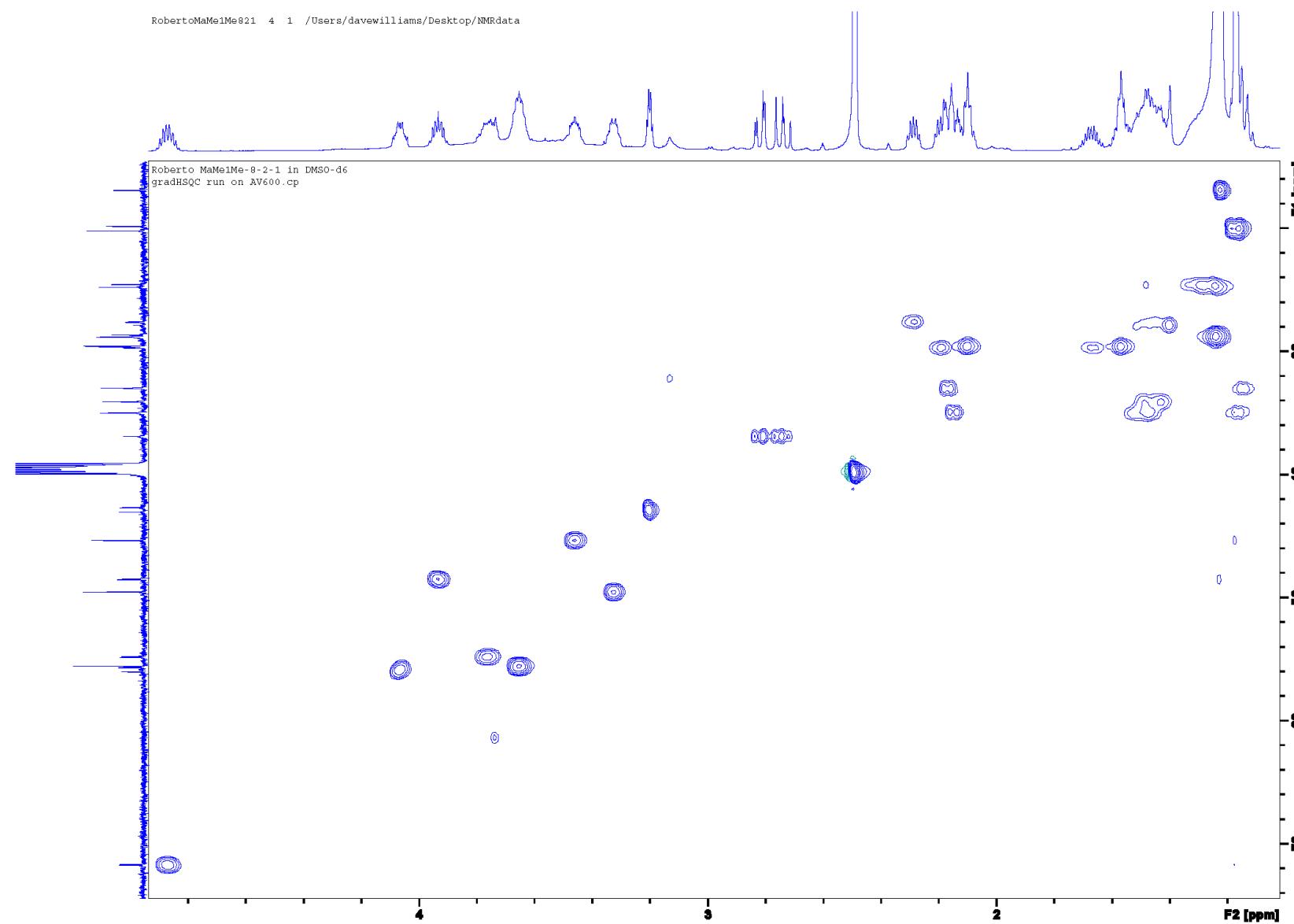


Figure S25. gHSQC spectrum (DMSO-*d*₆) of batzellamide A (**8**).

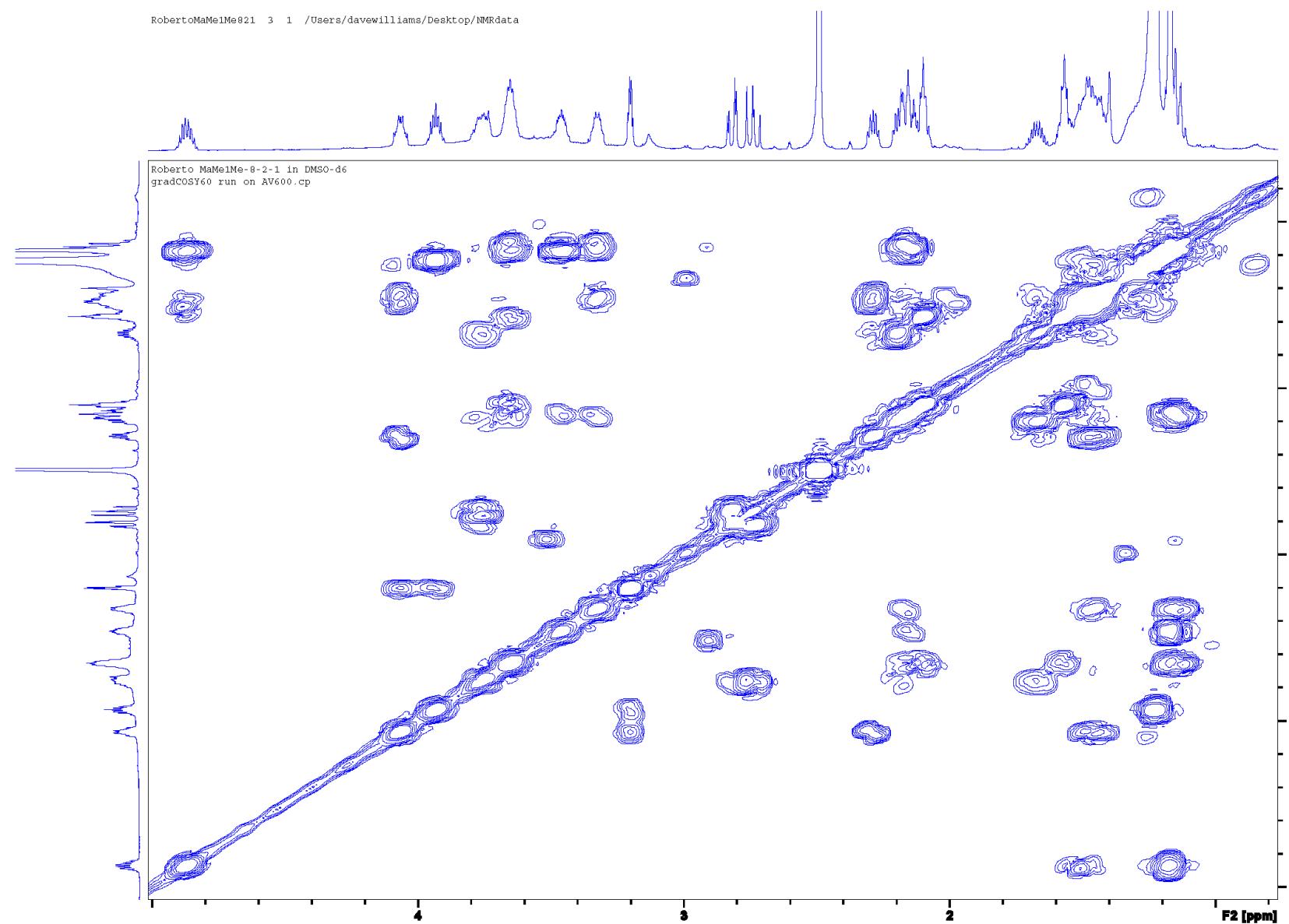


Figure S26. COSY spectrum (DMSO-*d*₆) of batzellamide A (**8**).

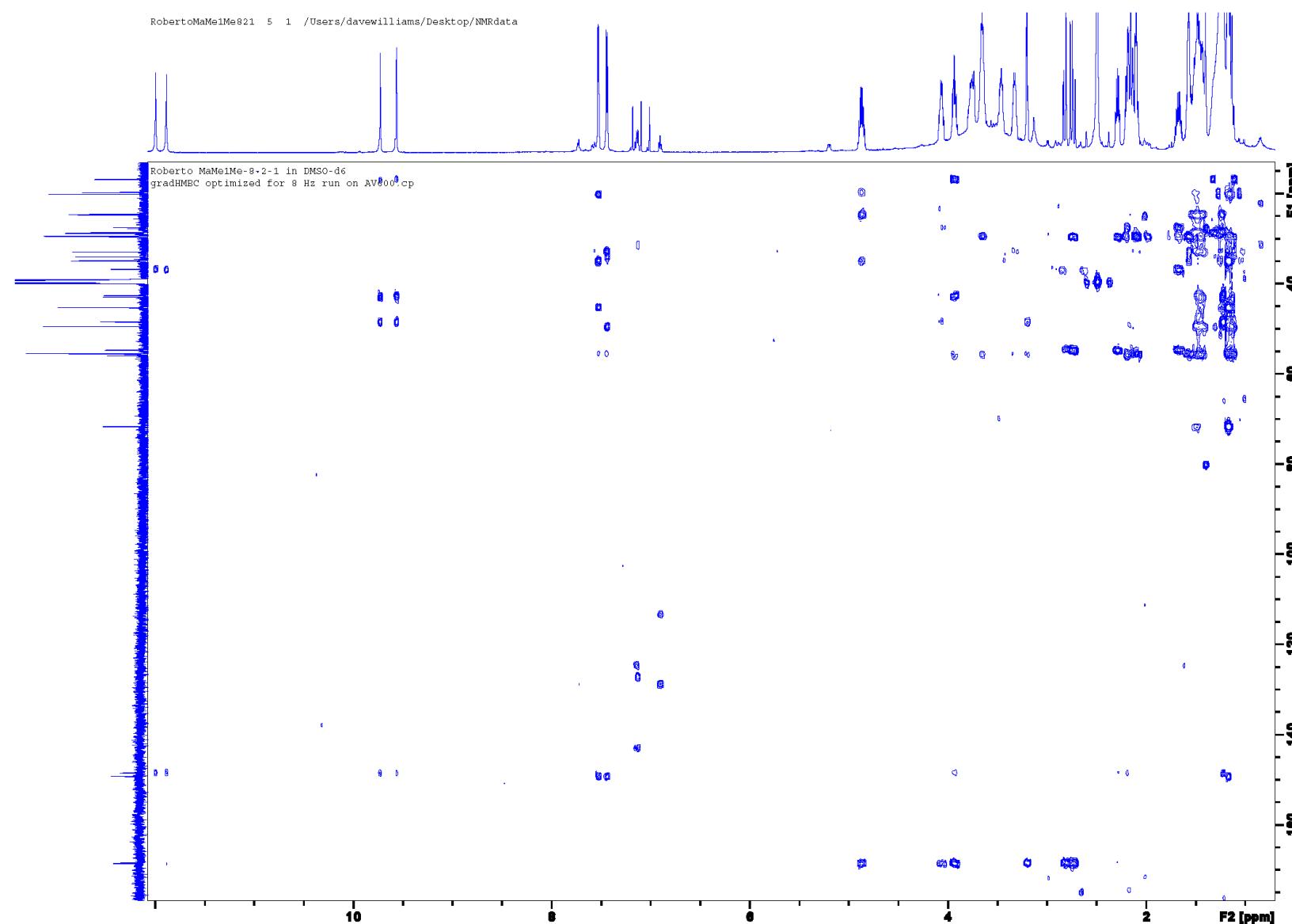


Figure S27. gHMBC spectrum (DMSO-*d*₆) of batzellamide A (**8**).

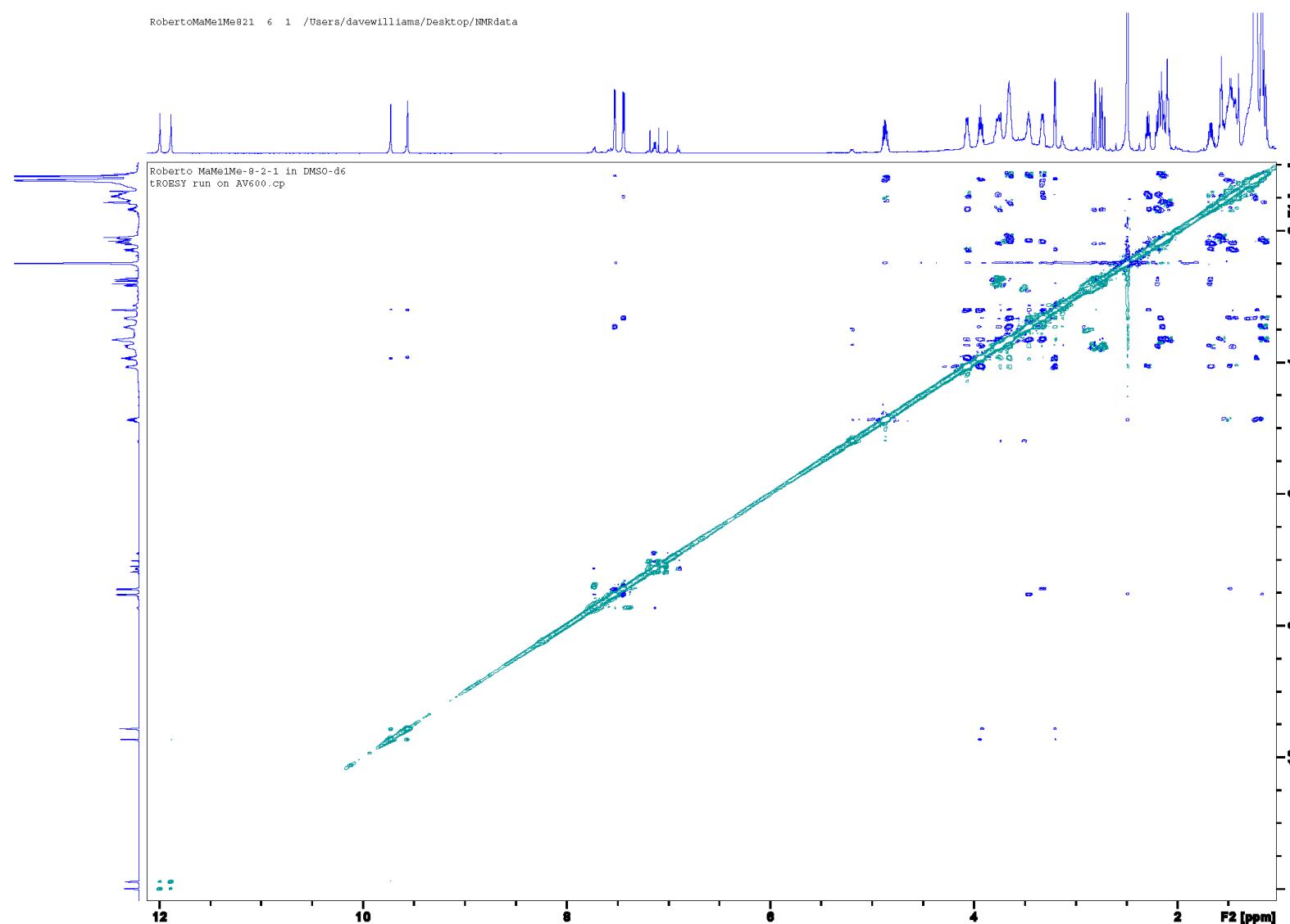


Figure S28. tROESY spectrum (DMSO-*d*₆) of batzellamide A (**8**).

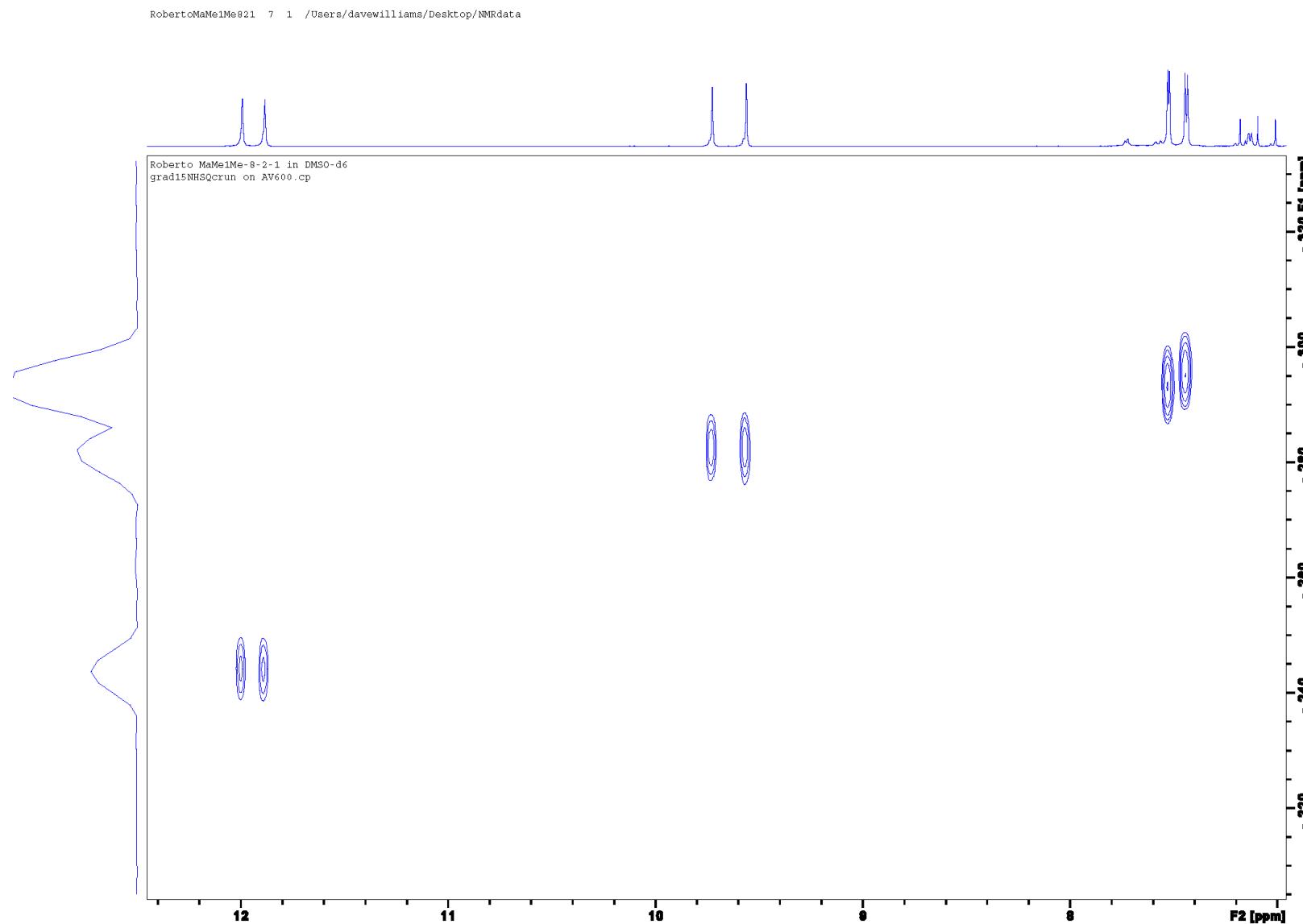


Figure S29. ¹⁵NHSQC spectrum (DMSO-*d*₆) of batzellamide A (**8**).

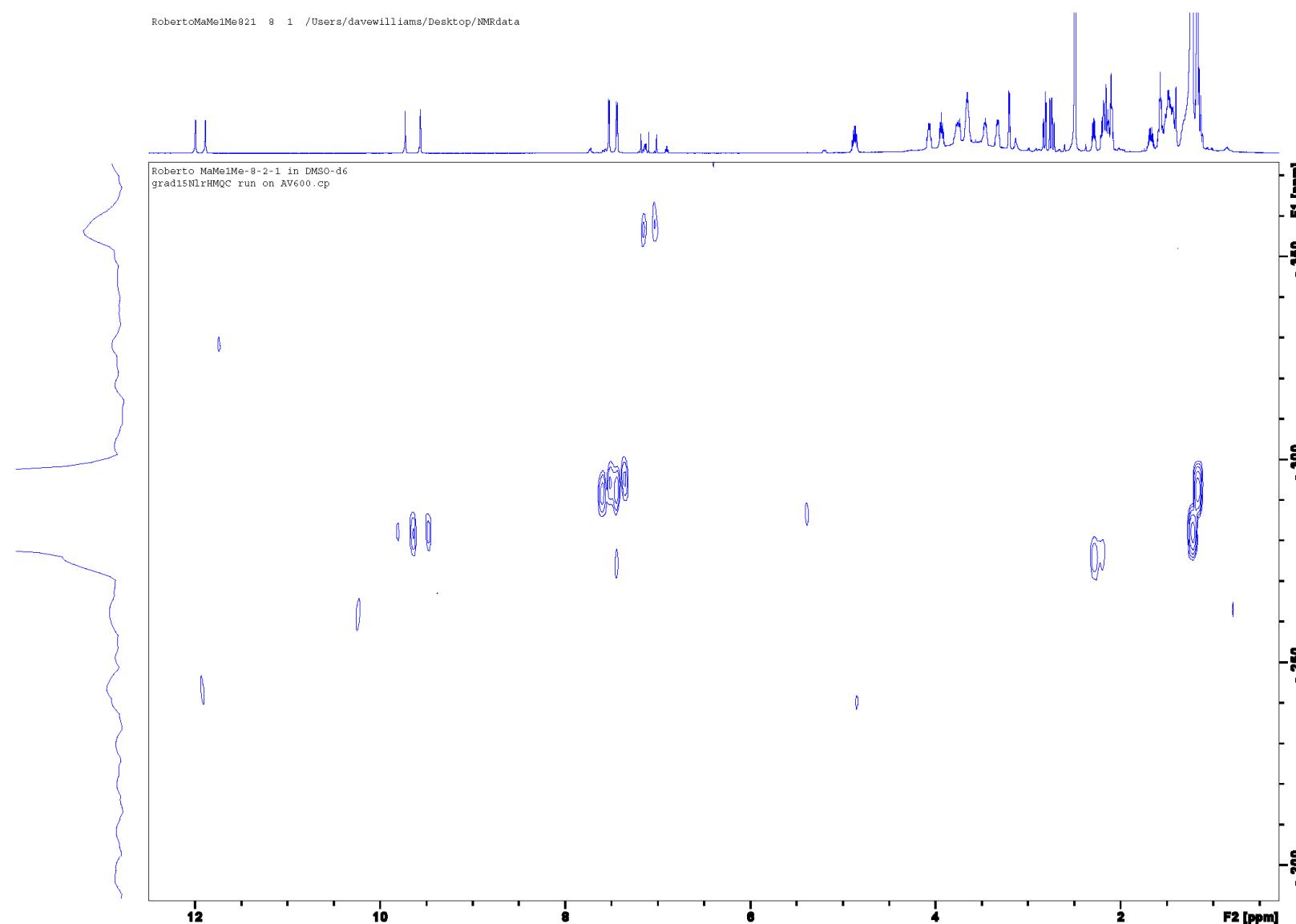


Figure S30. ¹⁵NLRHMQC spectrum (DMSO-*d*₆) of batzellamide A (**8**).

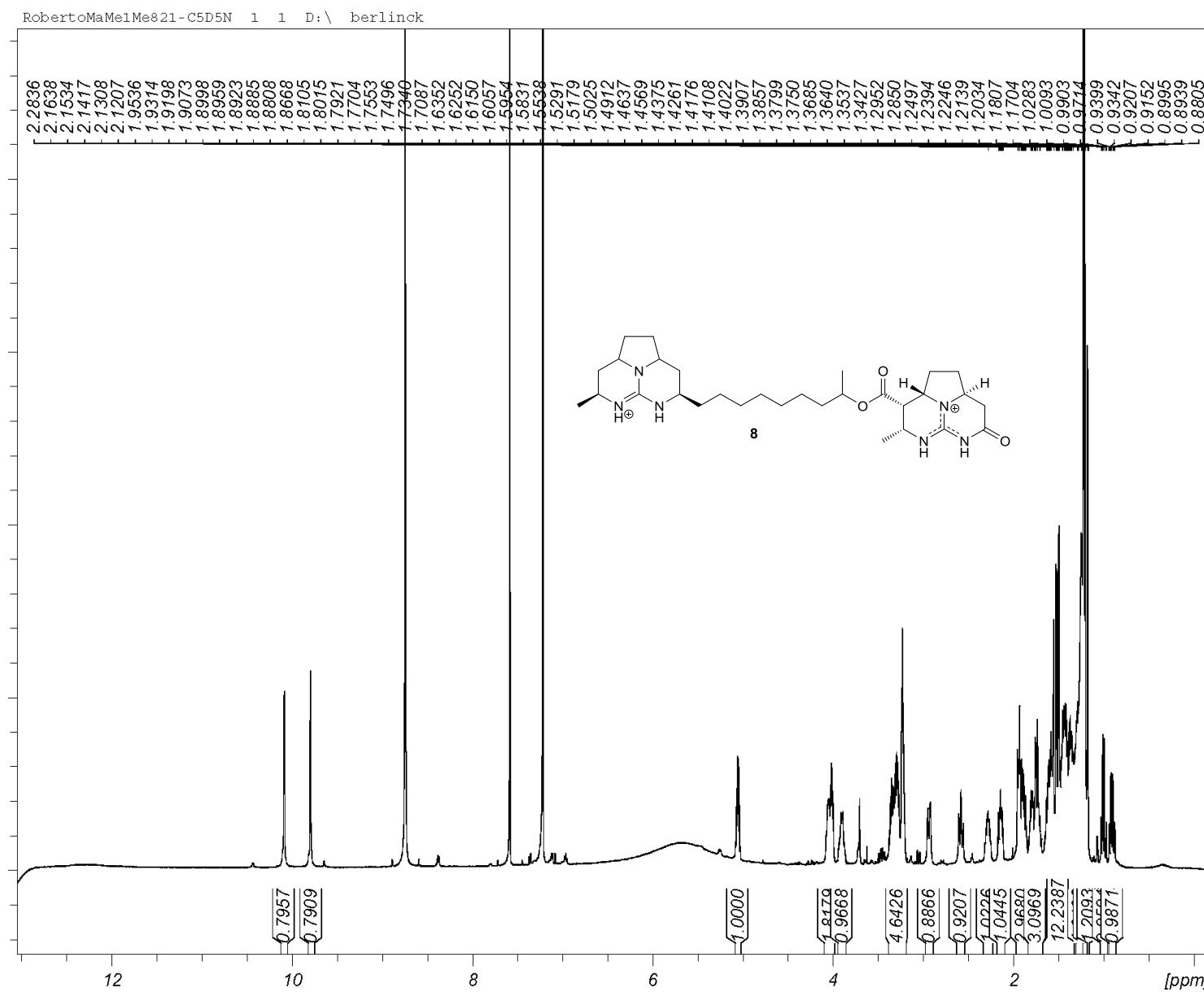


Figure S31. ^1H NMR spectrum (600 MHz, pyridine-*d*₅) of batzellamide A (**8**).

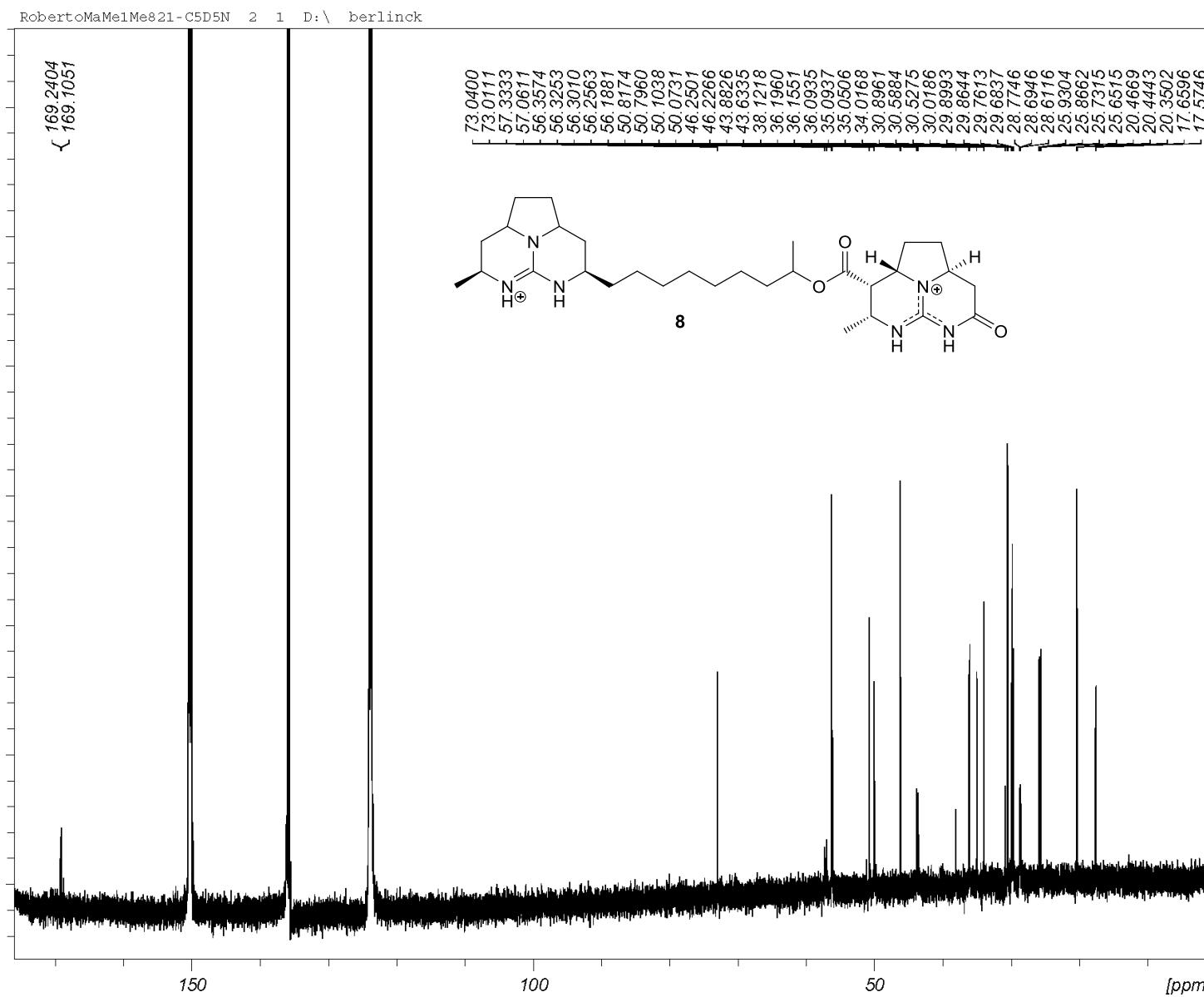


Figure S32. ^{13}C NMR spectrum (150 MHz, pyridine-*d*₅) of batzellamide A (**8**).

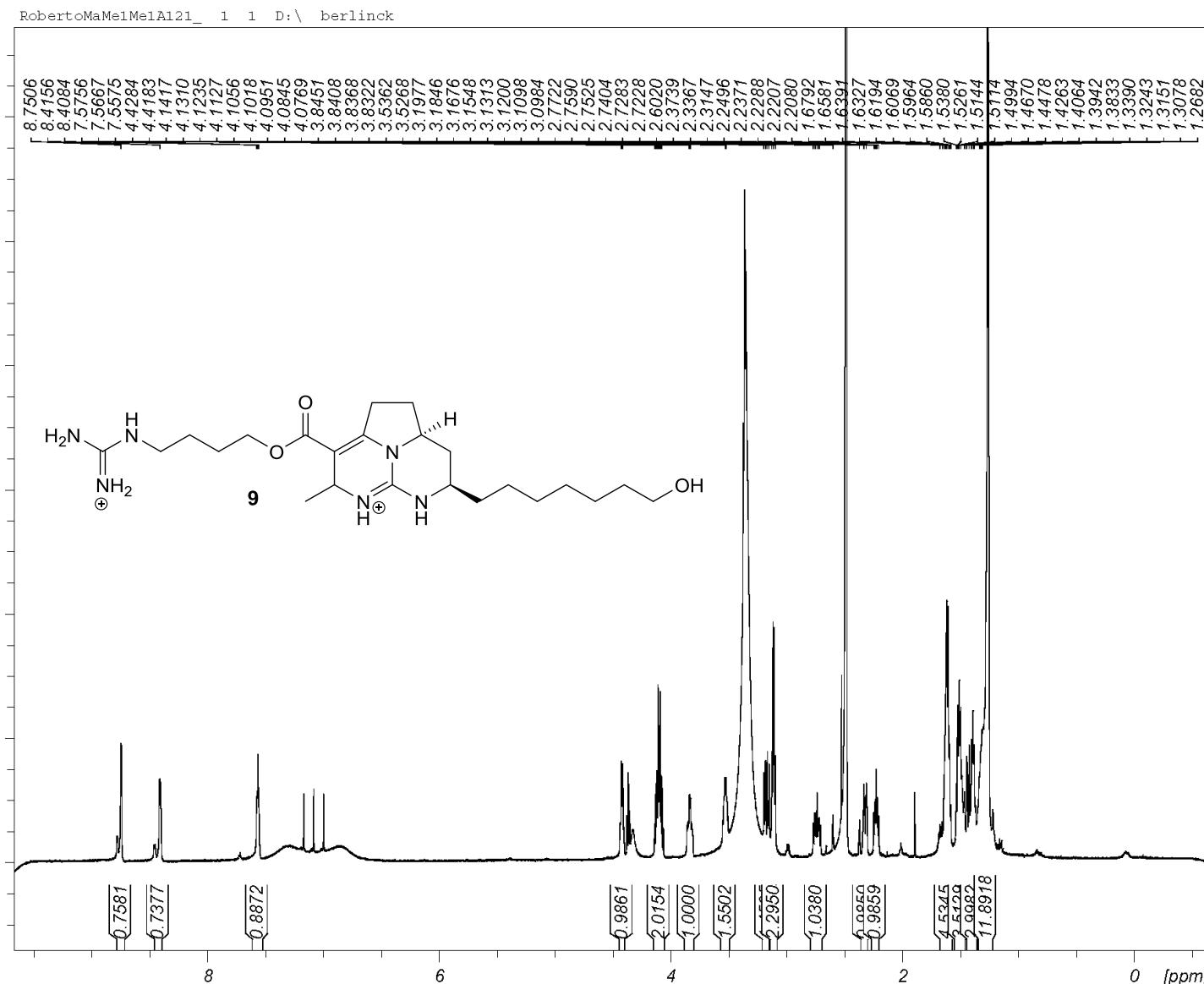


Figure S33. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of hemibatzzelladine J (**9**).

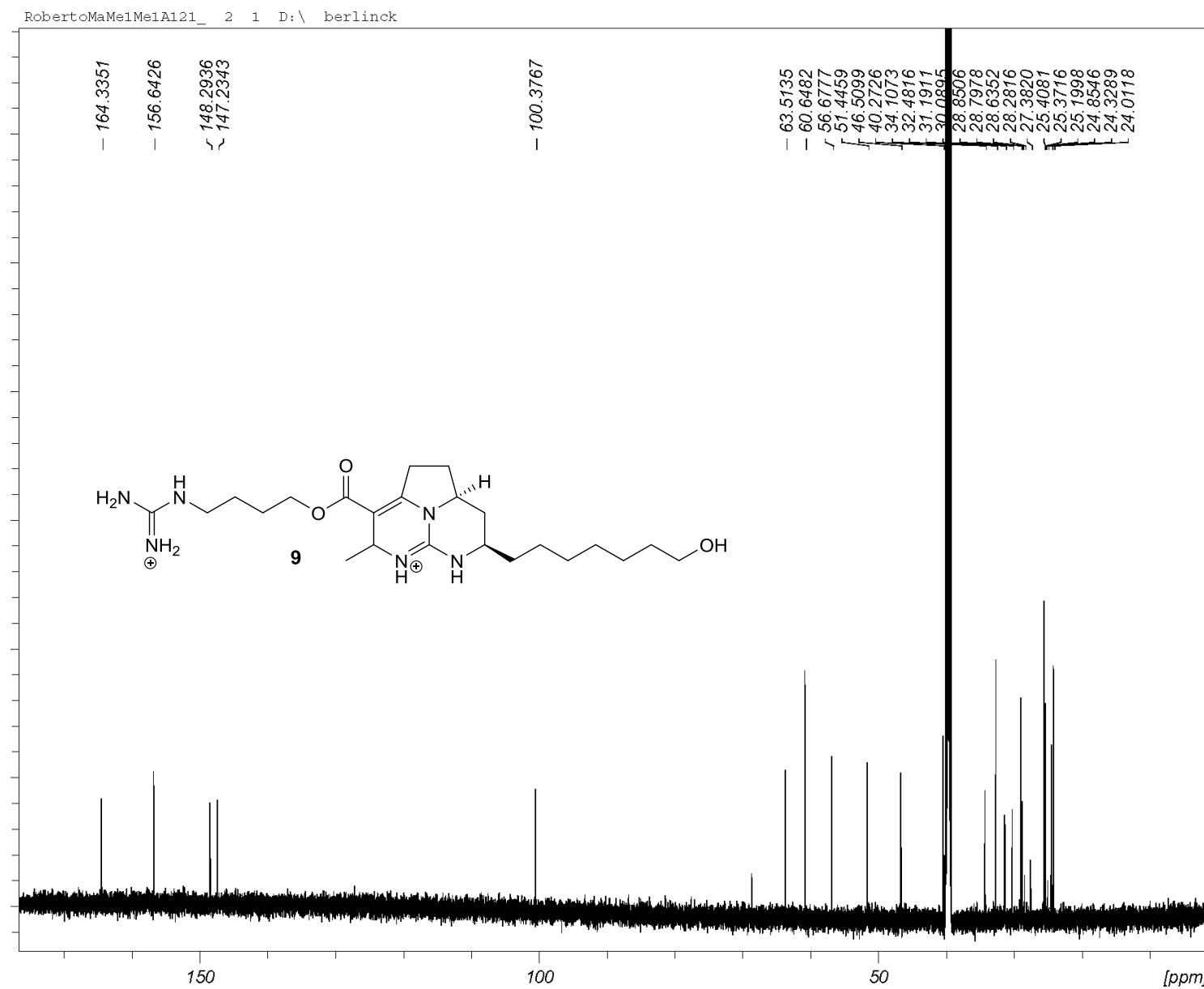


Figure S34. ¹H NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of hemibatzzelladine J (**9**).

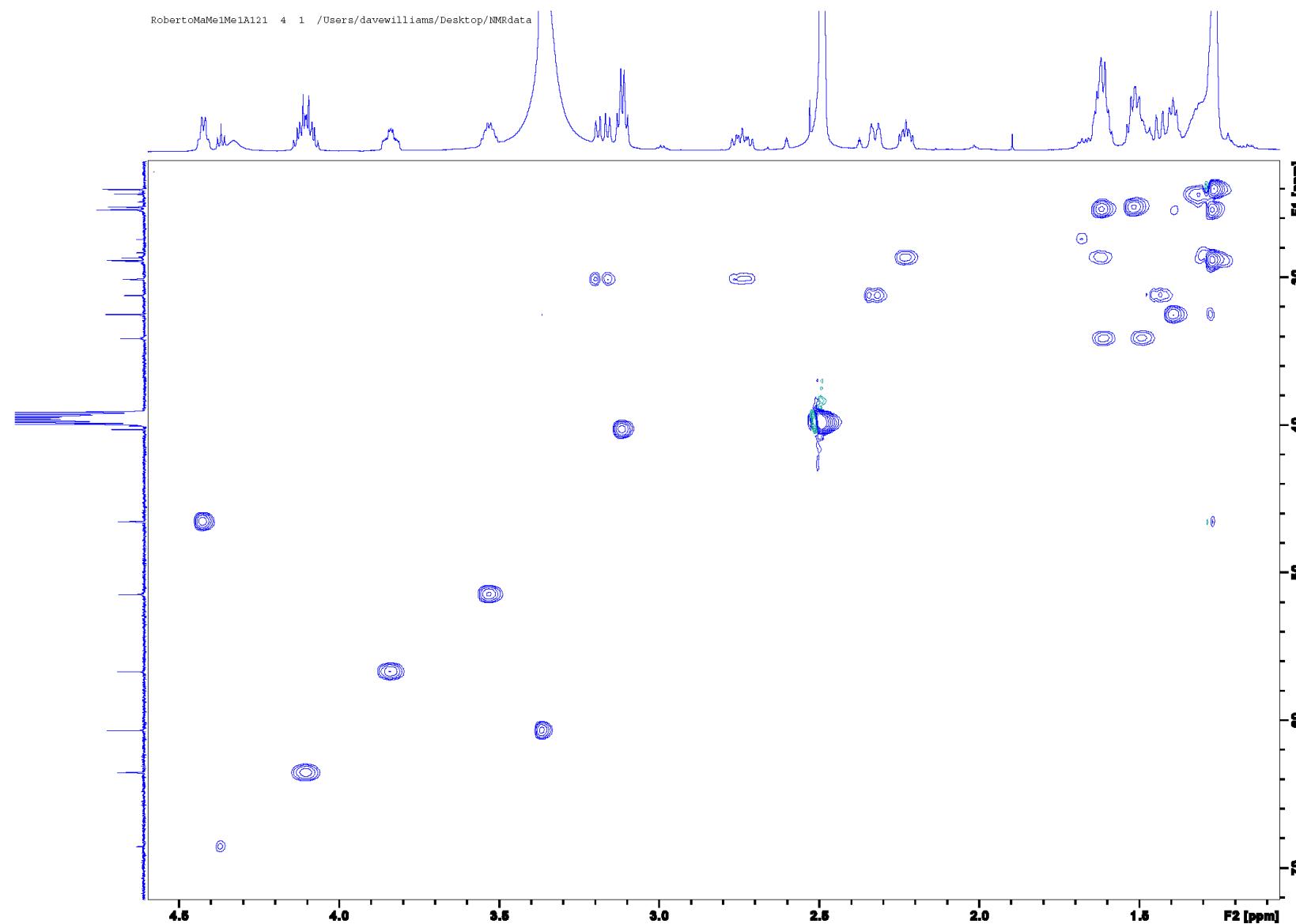


Figure S35. gHSQC spectrum ($\text{DMSO}-d_6$) of hemibatzzelladine J (**9**).

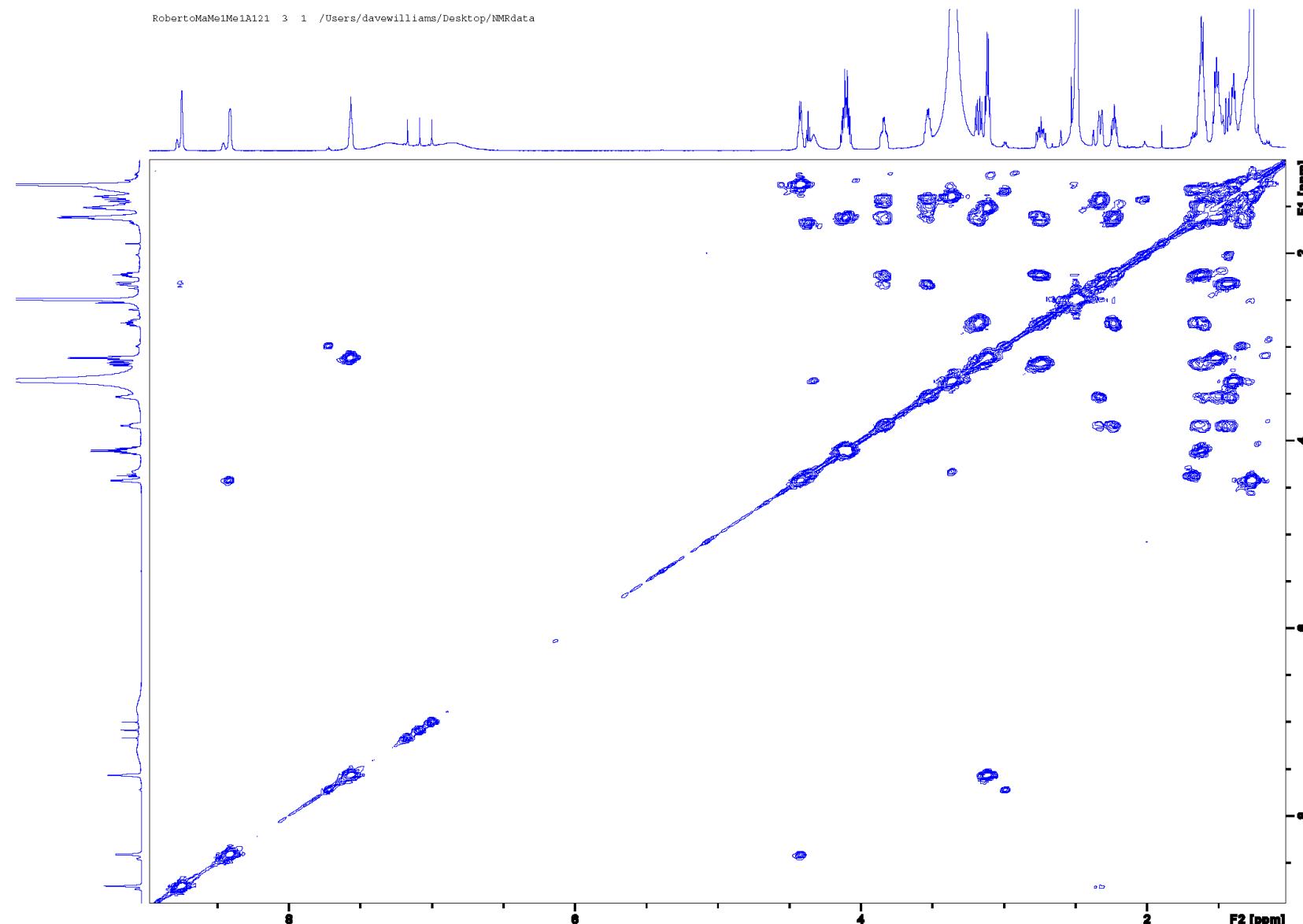


Figure S36. COSY spectrum ($\text{DMSO}-d_6$) of hemibatzelladine J (**9**).

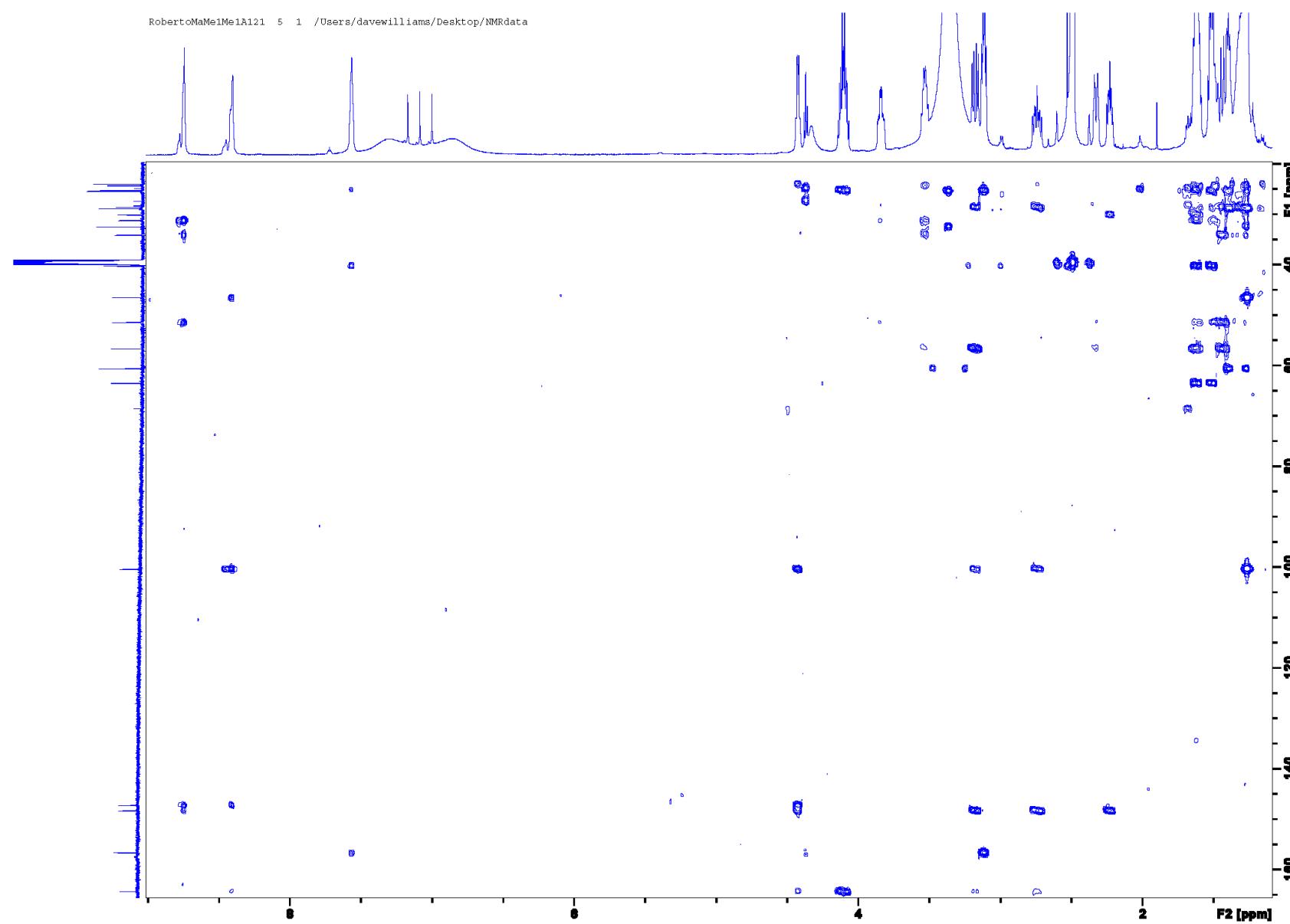


Figure S37. gHMBC spectrum ($\text{DMSO}-d_6$) of hemibatzelladine J (**9**).

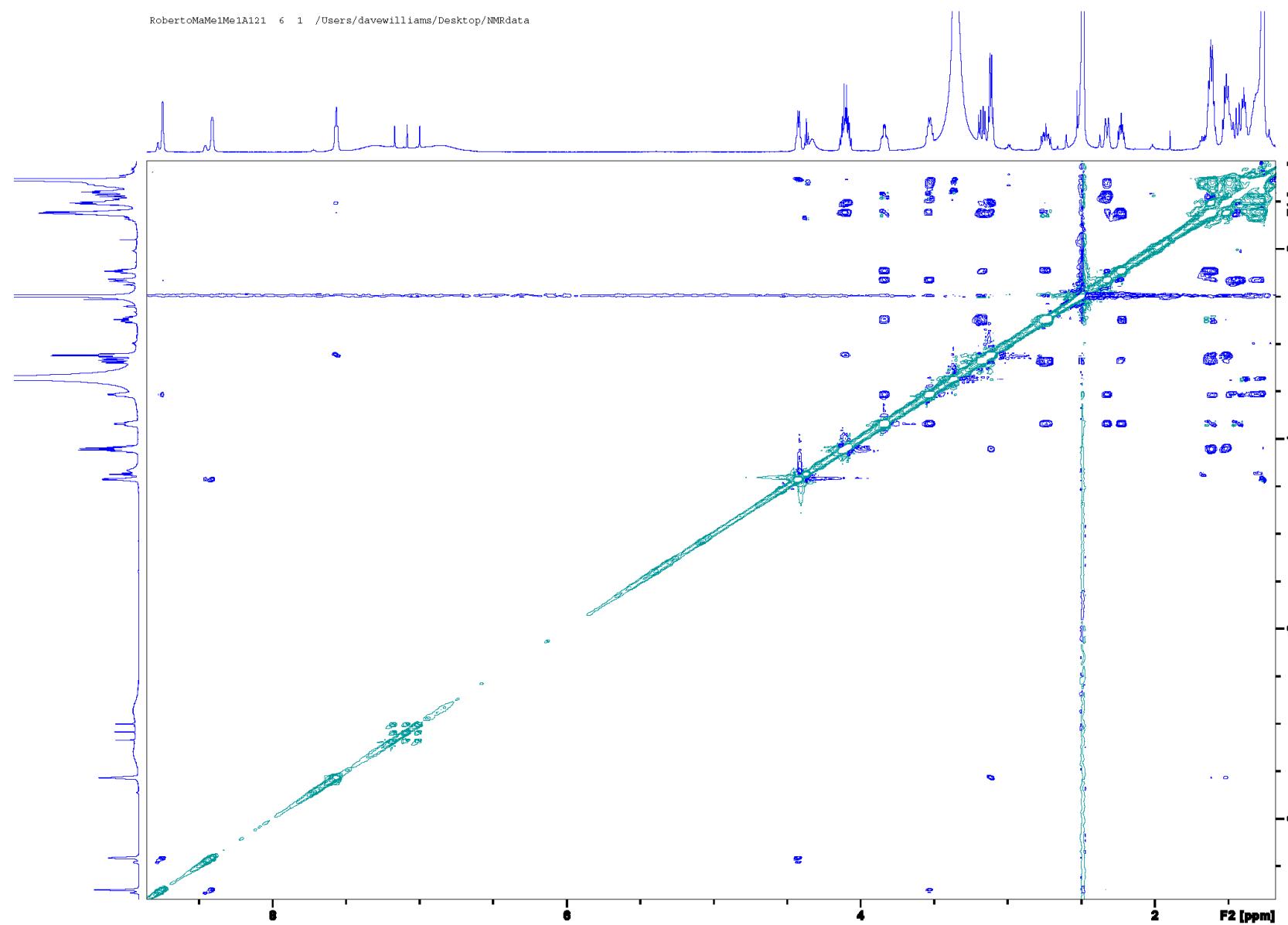


Figure S38. tROESY spectrum (DMSO-*d*₆) of hemibatzzelladine J (**9**).

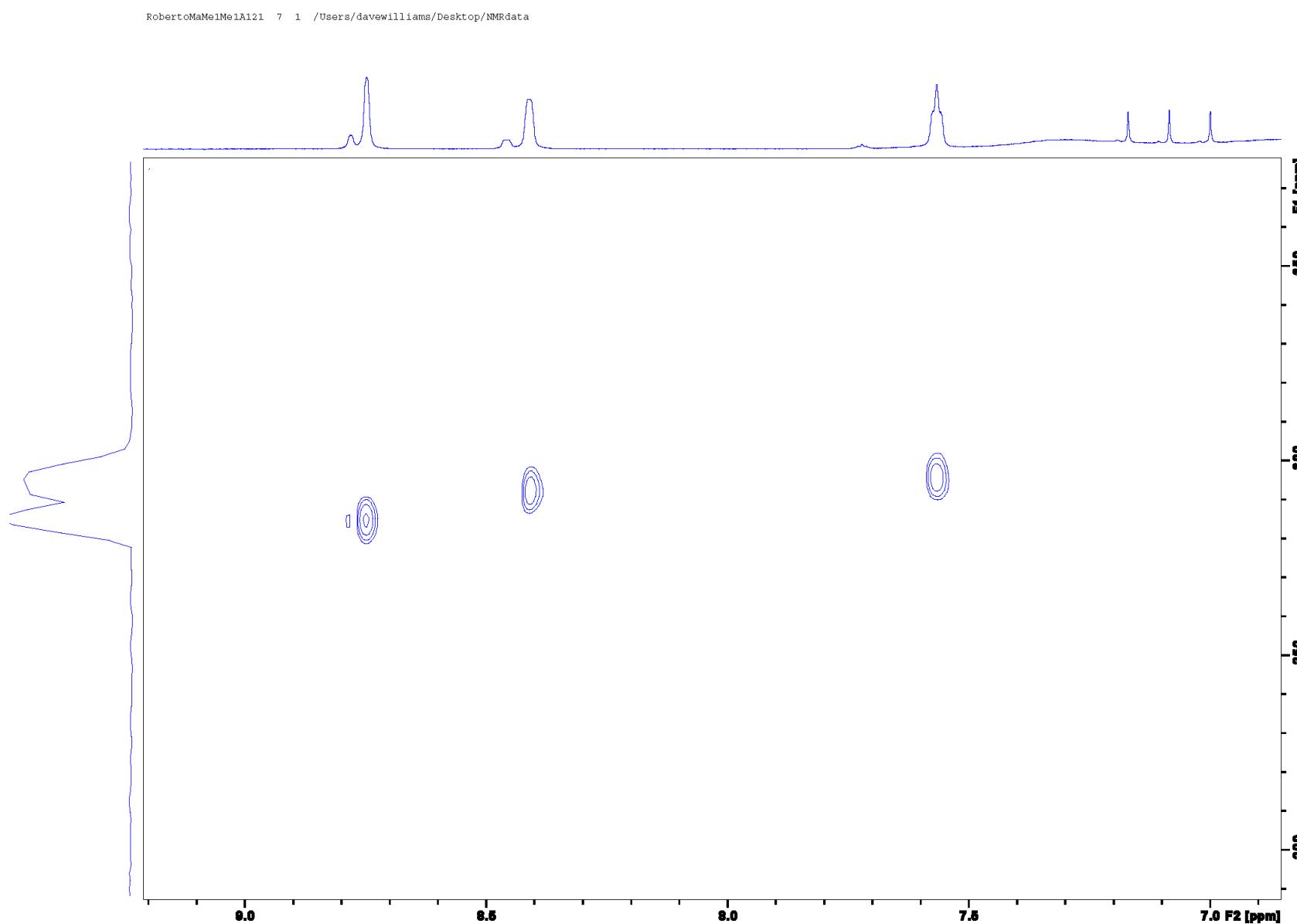


Figure S39. ^{15}N HSQC spectrum (DMSO- d_6) of hemibatzelladine J (**9**).

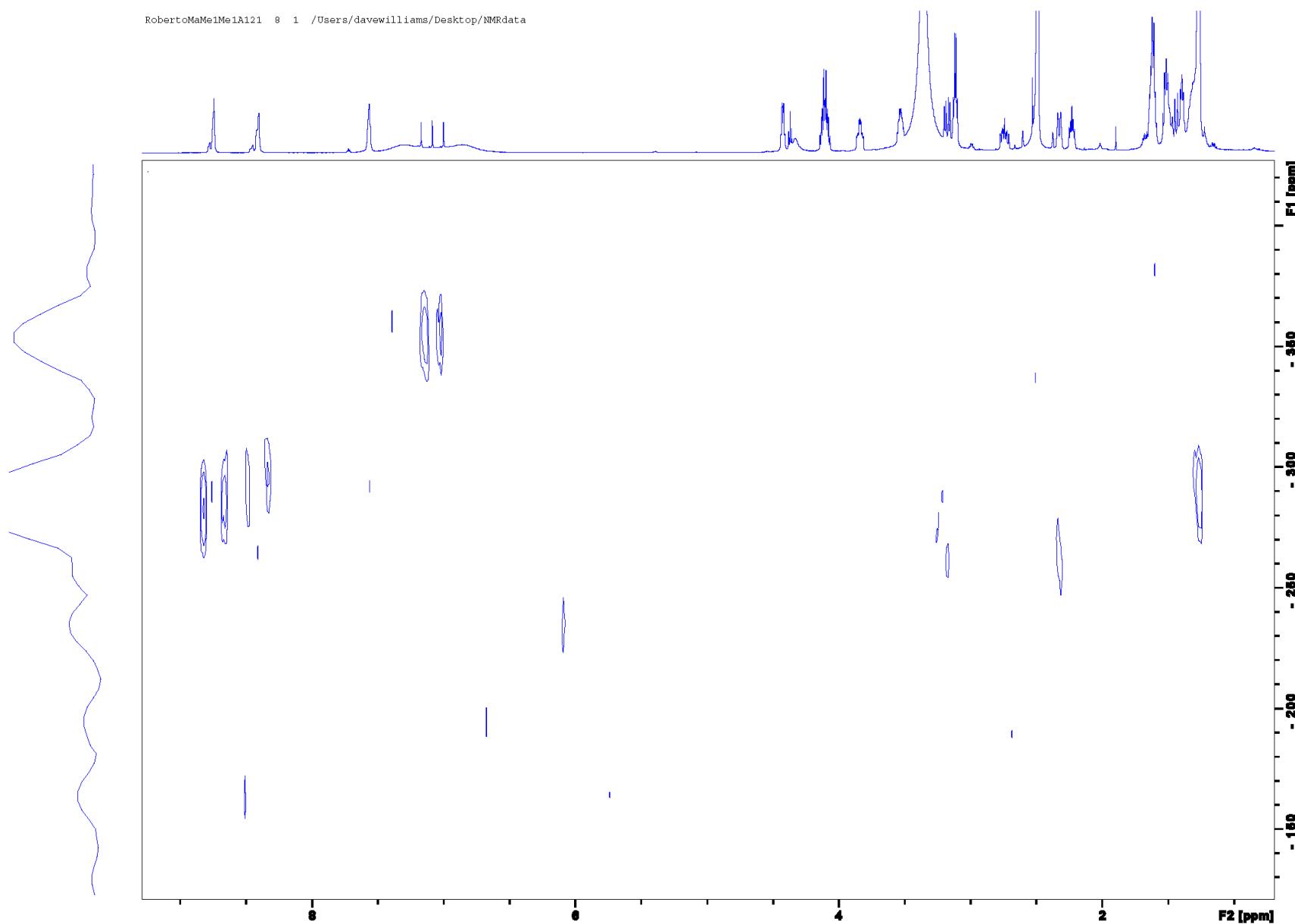


Figure S40. ¹⁵N-LRHMBC spectrum (DMSO-*d*₆) of hemibatzelladine J (**9**).

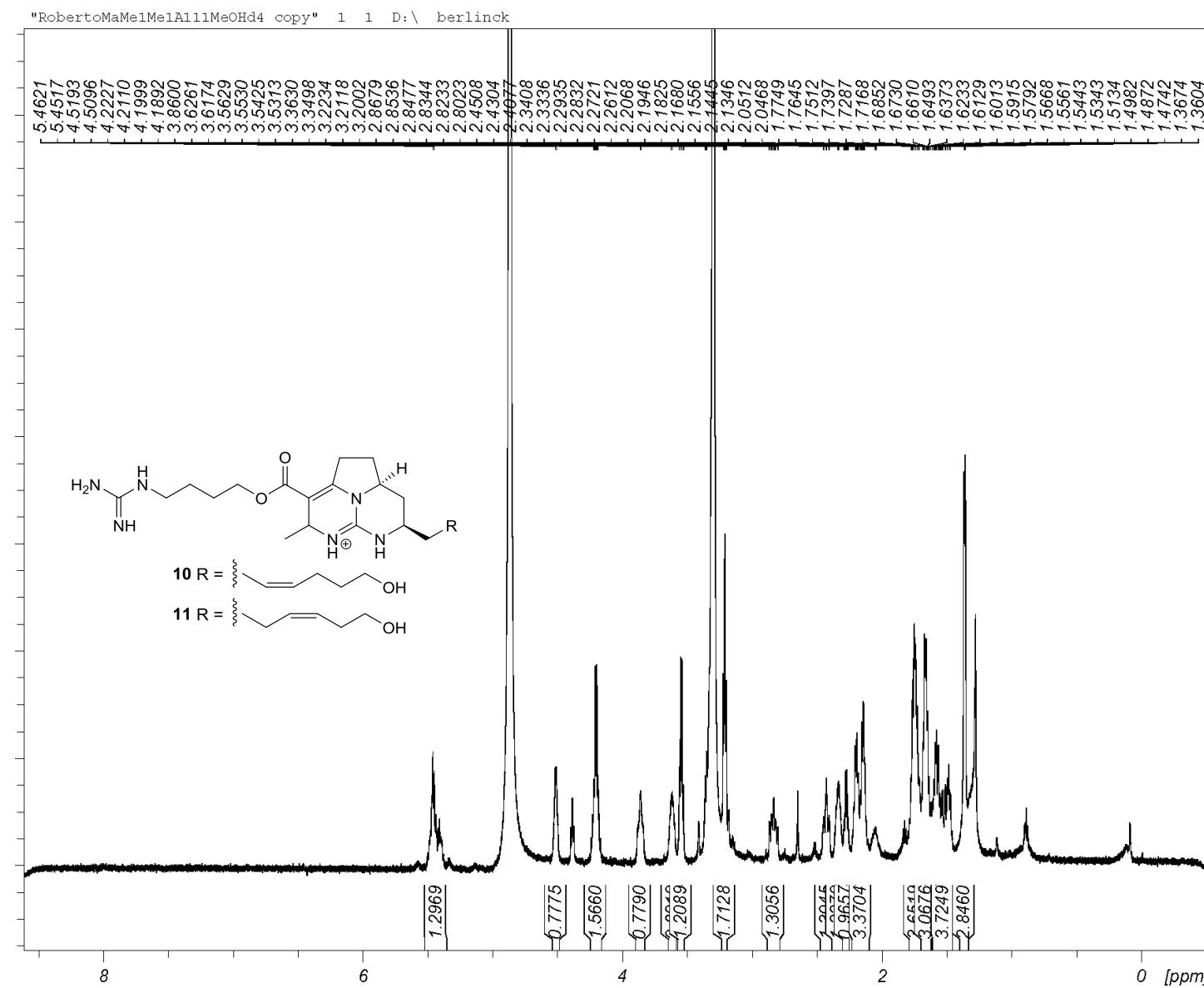


Figure S41. ^1H NMR spectrum (600 MHz, MeOH- d_4) of Δ^{19-20} -hemibatzzelladine J (**10**) and Δ^{20-21} -hemibatzzelladine J (**11**).

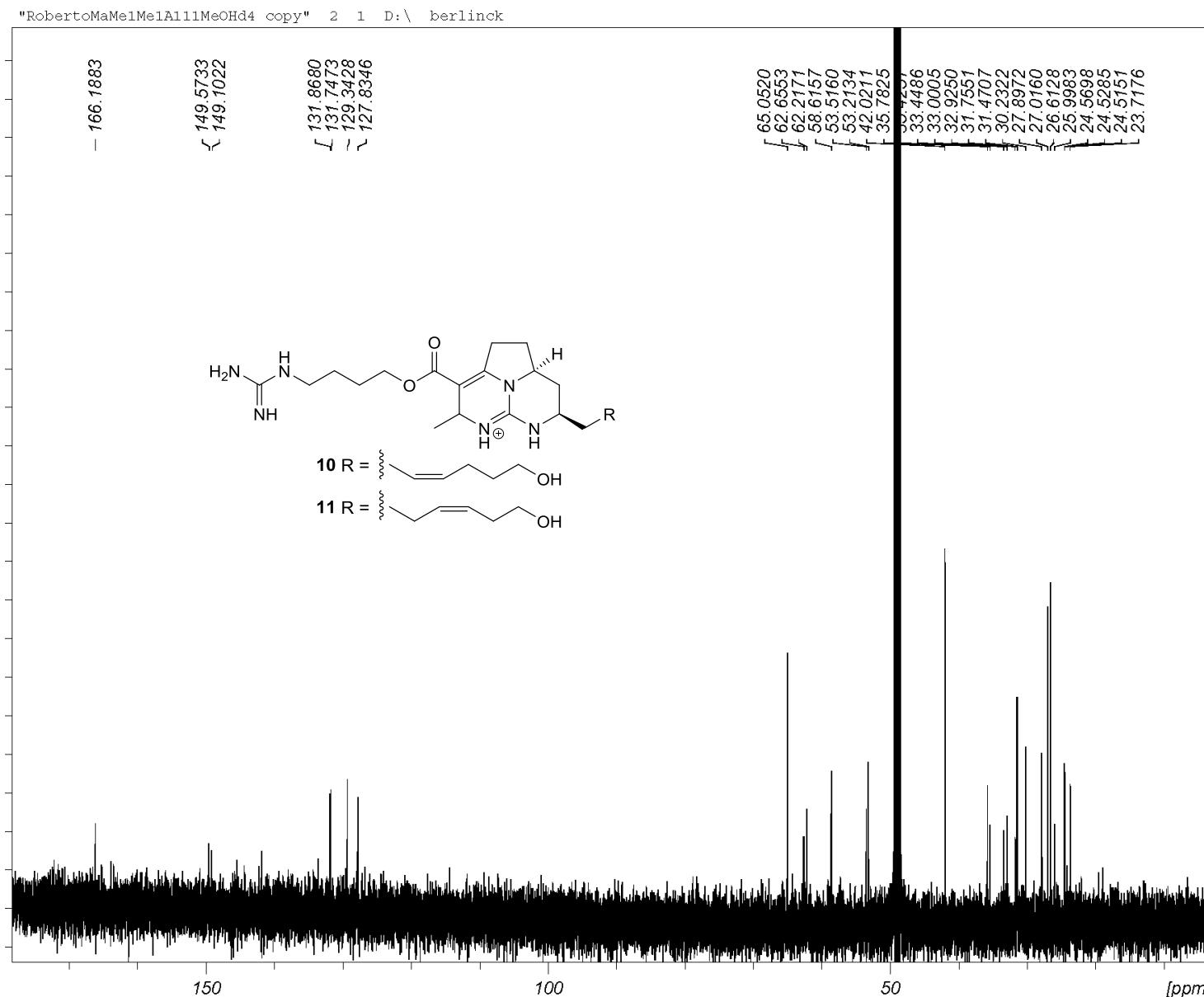


Figure S42. ^{13}C NMR spectrum (150 MHz, $\text{MeOH}-d_4$) of Δ^{19-20} -hemibatzelladine J (**10**) and Δ^{20-21} -hemibatzelladine J (**11**).

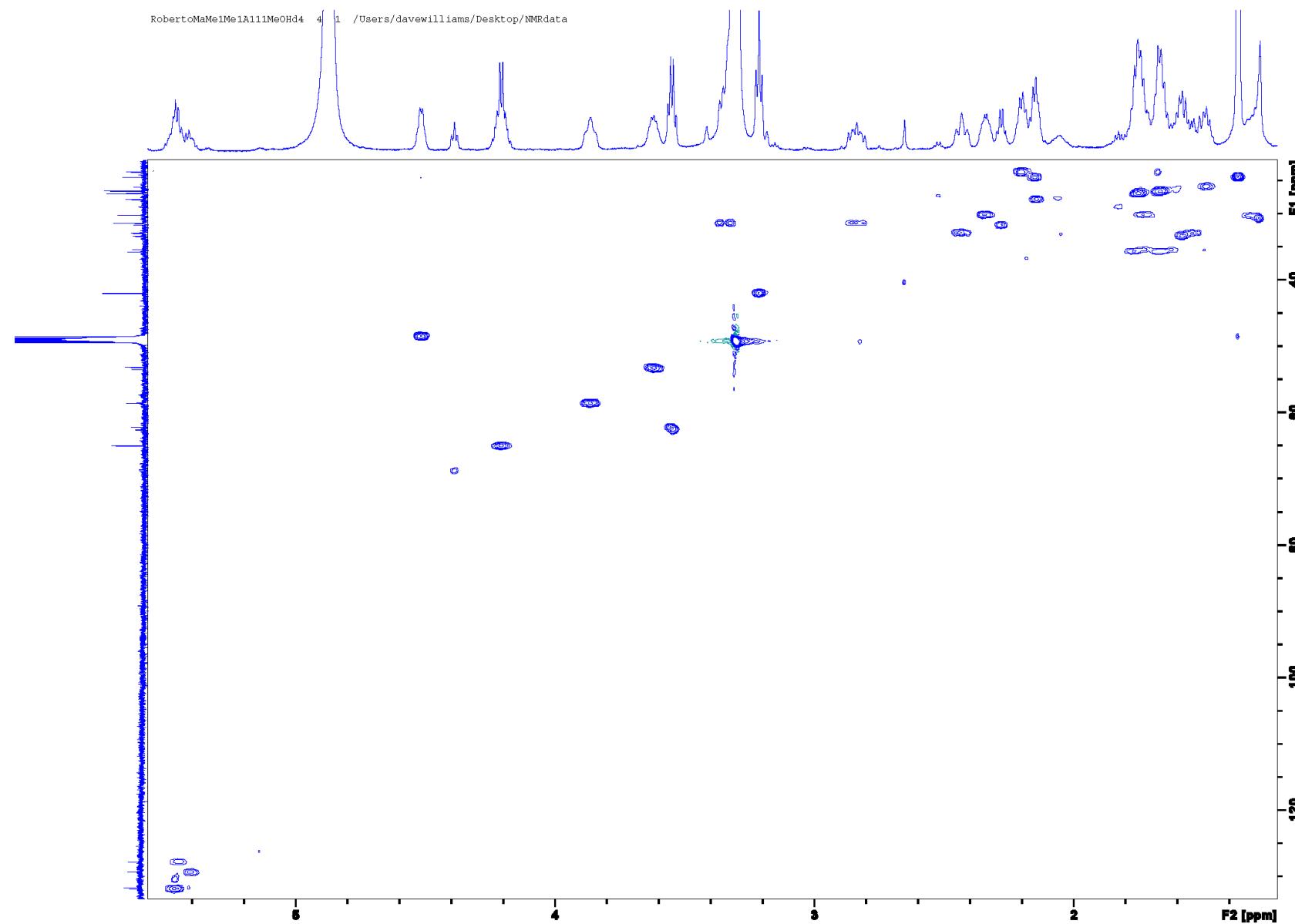


Figure S43. gHSQC spectrum ($\text{MeOH-}d_4$) of Δ^{19-20} -hemibatzelladine J (**10**) and Δ^{20-21} -hemibatzelladine J (**11**).

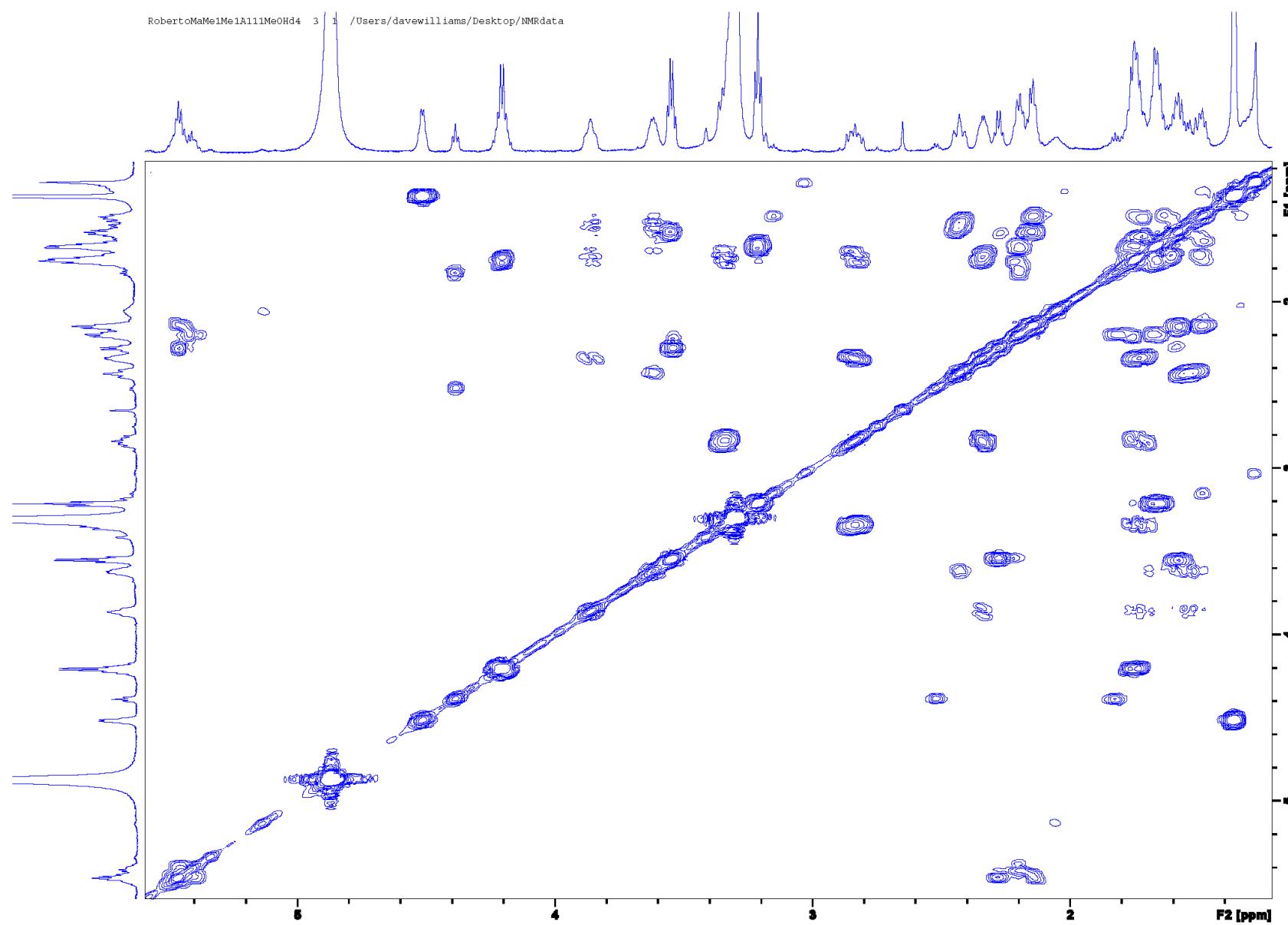


Figure S44. COSY spectrum ($\text{MeOH-}d_4$) of Δ^{19-20} -hemibatzelladine J (**10**) and Δ^{20-21} -hemibatzelladine J (**11**).

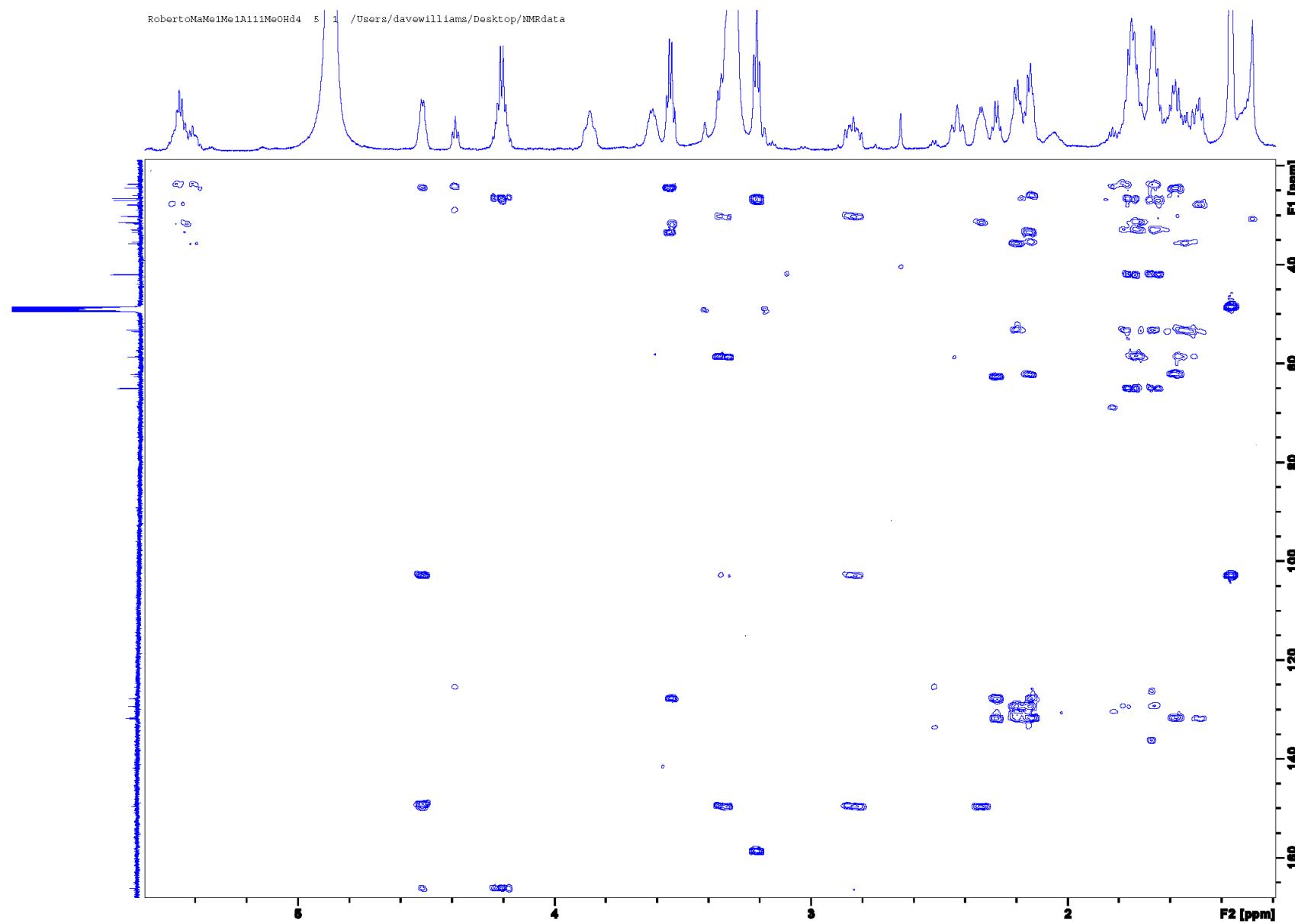


Figure S45. gHMBC spectrum ($\text{MeOH}-d_4$) of Δ^{19-20} -hemibatzelladine J (**10**) and Δ^{20-21} -hemibatzelladine J (**11**).

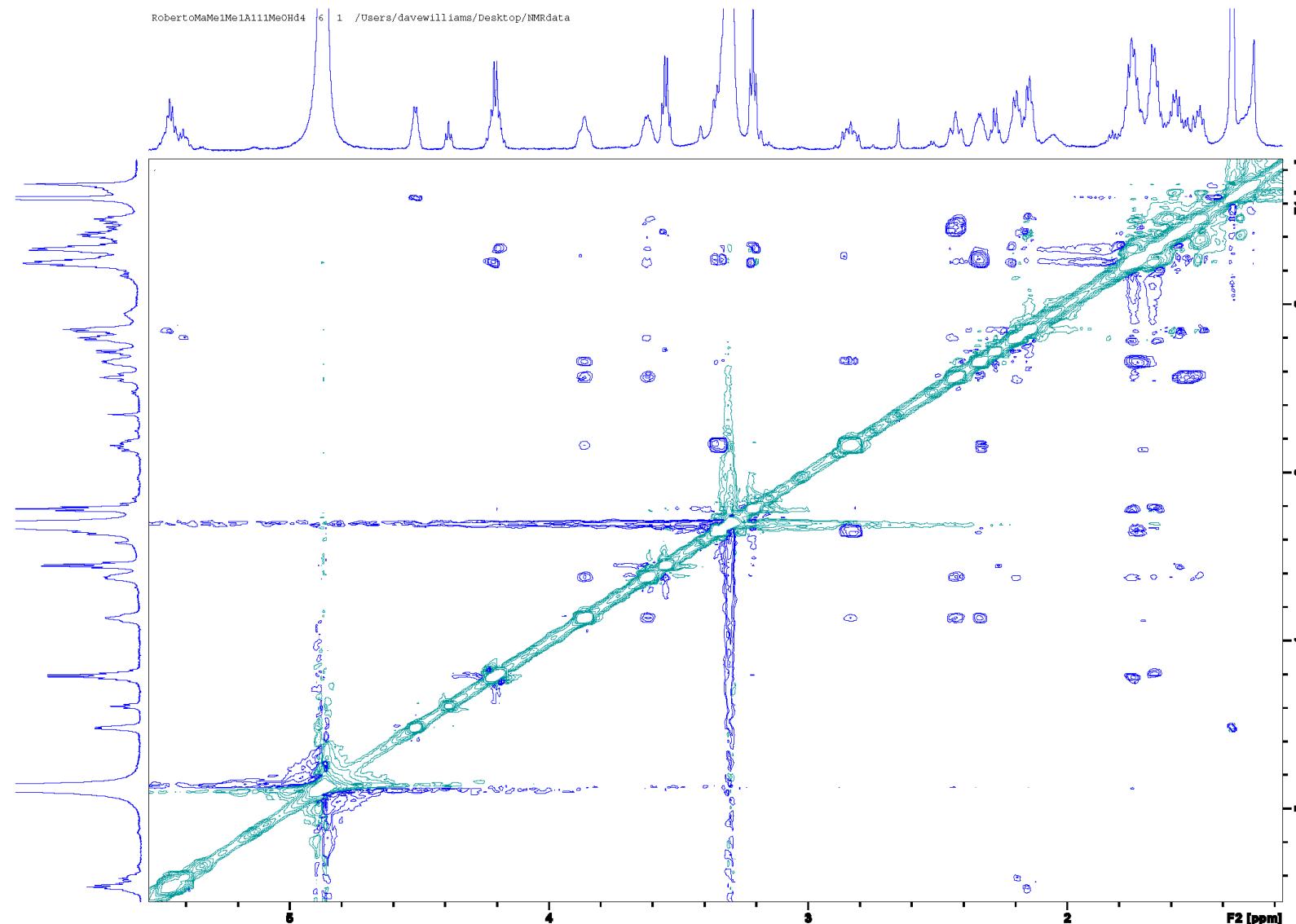


Figure S46. tROESY spectrum ($\text{MeOH}-d_4$) of Δ^{19-20} -hemibatzelladine **J** (**10**) and Δ^{20-21} -hemibatzelladine **J** (**11**).

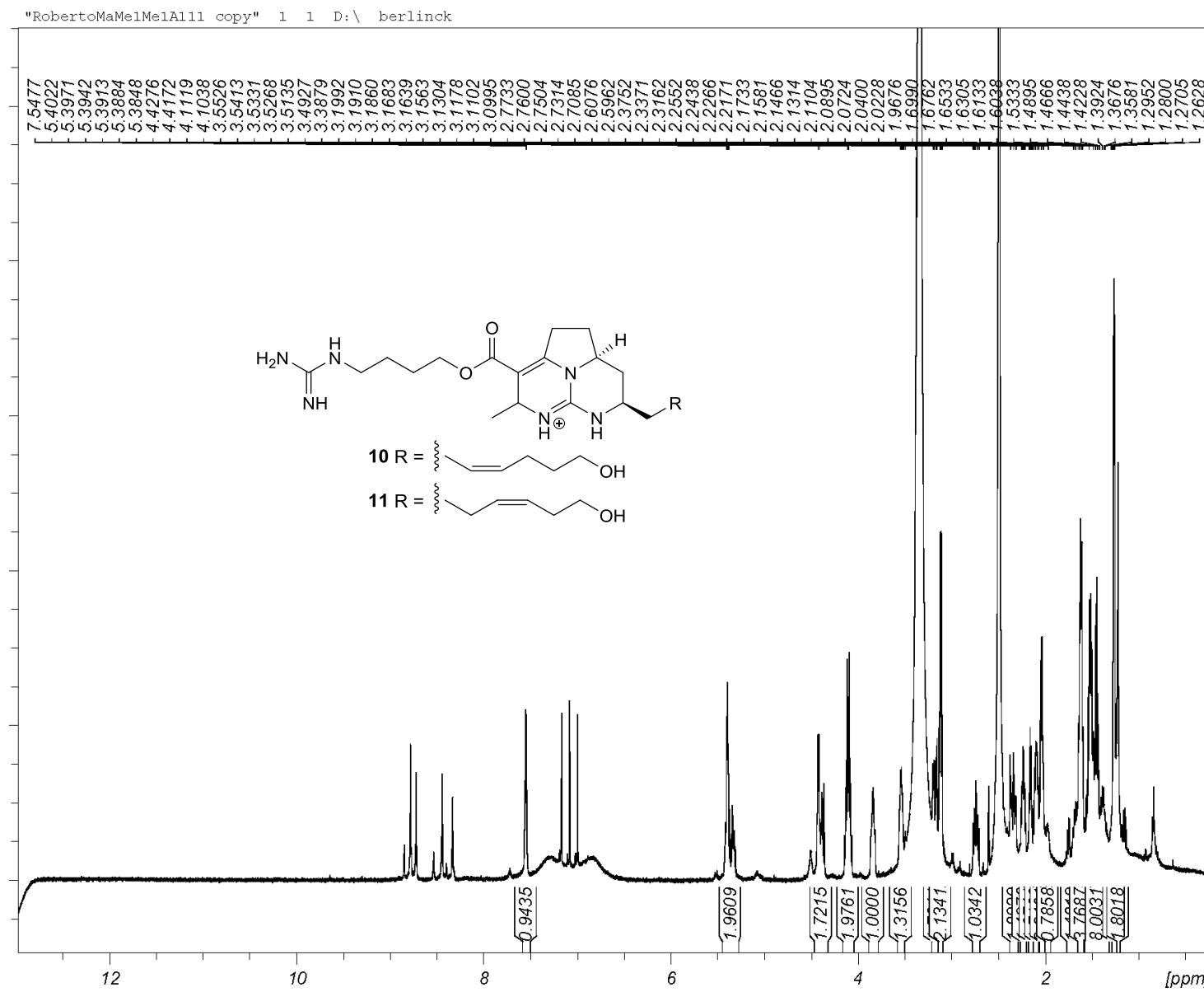


Figure S47. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_4$) of Δ^{19-20} -hemibatzelladine J (**10**) and Δ^{20-21} -hemibatzelladine J (**11**).

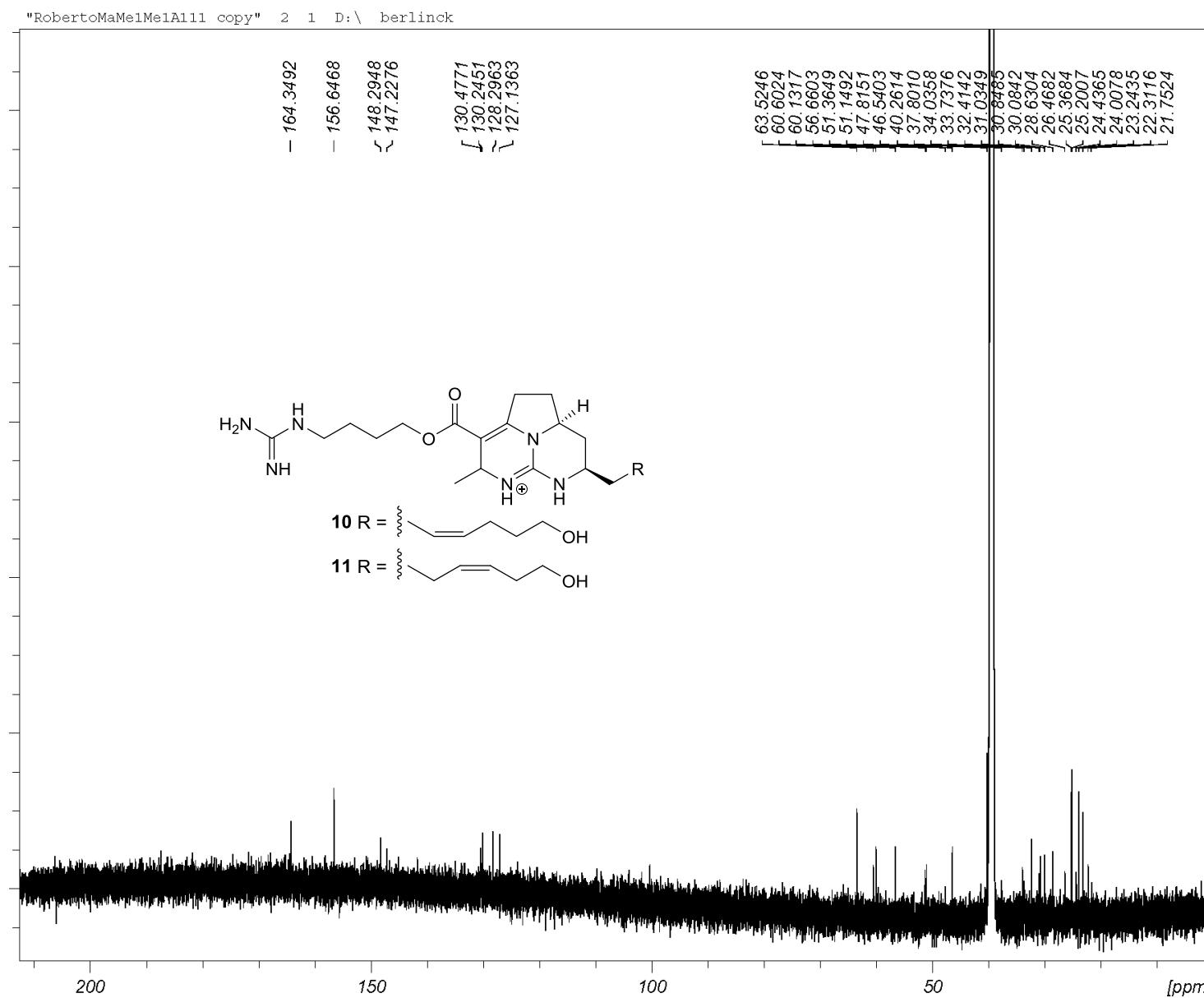


Figure S48. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_4$) of Δ^{19-20} -hemibatzelladine **J** (**10**) and Δ^{20-21} -hemibatzelladine **J** (**11**).