

Supporting information — part (II) of (IV)

Fine Tuning of Electrostatics Around the Internucleotidic Phosphate through Incorporation of Modified 2', 4'-Carbocyclic-LNA and –ENAs Leads to Significant Modulation of Antisense Properties

Chuanzheng Zhou, Yi Liu, Mounir Andaloussi, Naresh Badgujar, Oleksandr Plashkevych, Jyoti Chattopadhyaya*

Department of Bioorganic Chemistry, Box 581, Biomedical Center,

Uppsala University, SE-751 23 Uppsala, Sweden

jyoti@boc.uu.se

Table of contents

Figure SII.1. ¹ H NMR spectrum of compound 25.....	4
Figure SII.2. ¹³ C NMR spectrum of compound 25.....	5
Figure SII.3. ¹ H NMR spectrum of compound 27.....	6
Figure SII.4. ¹³ C NMR spectrum of compound 27.....	7
Figure SII.5. ¹ H NMR spectrum of compound 28.....	8
Figure SII.6. ¹³ C NMR spectrum of compound 28.....	9
Figure SII.7. ¹ H NMR spectrum of compound 29.....	10
Figure SII.8. ¹³ C NMR spectrum of compound 29.....	11
Figure SII.9. ¹ H NMR spectrum of compound 30.....	12
Figure SII.10. ¹³ C NMR spectrum of compound 30.....	13
Figure SII.11. COSY spectrum of compound 30.....	14
Figure SII.12. HMQC spectrum of compound 30.	15

Figure SII.13. HMBC spectrum of compound 30.....	16
Figure SII.14. ^1H NMR spectrum of compound 31.....	17
Figure SII.15. ^{13}C NMR spectrum of compound 31.....	18
Figure SII.16. COSY spectrum of compound 31.....	19
Figure SII.17. HMQC spectrum of compound 31.	20
Figure SII.18. ^1H NMR spectrum of compound 32.....	21
Figure SII.19. ^{13}C NMR spectrum of compound 32.....	22
Figure SII.20. ^1H NMR spectrum of compound 33.....	23
Figure SII.21. ^{13}C NMR spectrum of compound 33.....	24
Figure SII.22. COSY spectrum of compound 33.....	25
Figure SII.23. HMQC spectrum of compound 33.	26
Figure SII.24. HMBC spectrum of compound 33.....	27
Figure SII.25. ^1H NMR spectrum of compound 34.....	28
Figure SII.26. ^{13}C NMR spectrum of compound 34.....	29
Figure SII.27. COSY spectrum of compound 34.....	30
Figure SII.28. HMQC spectrum of compound 34.	31
Figure SII.29. HMBC spectrum of compound 34.....	32
Figure SII.30. ^1H NMR spectrum of compound 35a.	33
Figure SII.31. ^{13}C NMR spectrum of compound 35a.	34
Figure SII.32. COSY spectrum of compound 35a.....	35
Figure SII.33. HMQC spectrum of compound 35a.....	36
Figure SII.34. HMBC spectrum of compound 35a.....	37
Figure SII.35. ^1H NMR spectrum of compound 35b.....	38
Figure SII.36. ^{13}C NMR spectrum of compound 35b.....	39
Figure SII.37. COSY spectrum of compound 35b.....	40
Figure SII.38. HMQC spectrum of compound 35b.	41
Figure SII.39. HMBC spectrum of compound 35b.....	42
Figure SII.40. ^1H NMR spectrum of compound 36.....	43
Figure SII.41. ^{13}C NMR spectrum of compound 36.....	44
Figure SII.42. COSY spectrum of compound 36.....	45
Figure SII.43. HMQC spectrum of compound 36.	46
Figure SII.44. HMBC spectrum of compound 36.....	47
Figure SII.45. ^1H NMR spectrum of compound 37.....	48

Figure SII.46. ^{13}C NMR spectrum of compound 37.....	49
Figure SII.47. ^1H NMR spectrum of compound 38.....	50
Figure SII.48. ^{13}C NMR spectrum of compound 38.....	51
Figure SII.49. ^1H NMR spectrum of compound 39.....	52
Figure SII.50. ^{13}C NMR spectrum of compound 39.....	53
Figure SII.51. ^1H NMR spectrum of compound 40.....	54
Figure SII.52. ^{13}C NMR spectrum of compound 40.....	55
Figure SII.53. ^1H NMR spectrum of compound 41.....	56
Figure SII.54. ^{13}C NMR spectrum of compound 41.....	57
Figure SII.55. ^1H NMR spectrum of compound 42.....	58
Figure SII.56. ^{13}C NMR spectrum of compound 42.....	59
Figure SII.57. ^1H NMR spectrum of compound 43.....	60
Figure SII.58. ^{13}C NMR spectrum of compound 43.....	61
Figure SII.59. ^{31}P NMR spectrum of compound 44.....	62
Figure SII.60. ^{31}P NMR spectrum of compound 45.....	63
Figure SII.61. ^{31}P NMR spectrum of compound 46.....	64
Figure SII.62. ^1H and $^1\text{H} \{^{31}\text{P}\}$ NMR spectrum of compound 46 (isomer I).....	65
Figure SII.63. ^1H and $^1\text{H} \{^{31}\text{P}\}$ NMR spectrum of compound 46 (isomer II).....	65
Figure SII.64. ^{31}P NMR spectrum of compound 47.....	66
Figure SII.65. ^{31}P NMR spectrum of compound 48.....	67

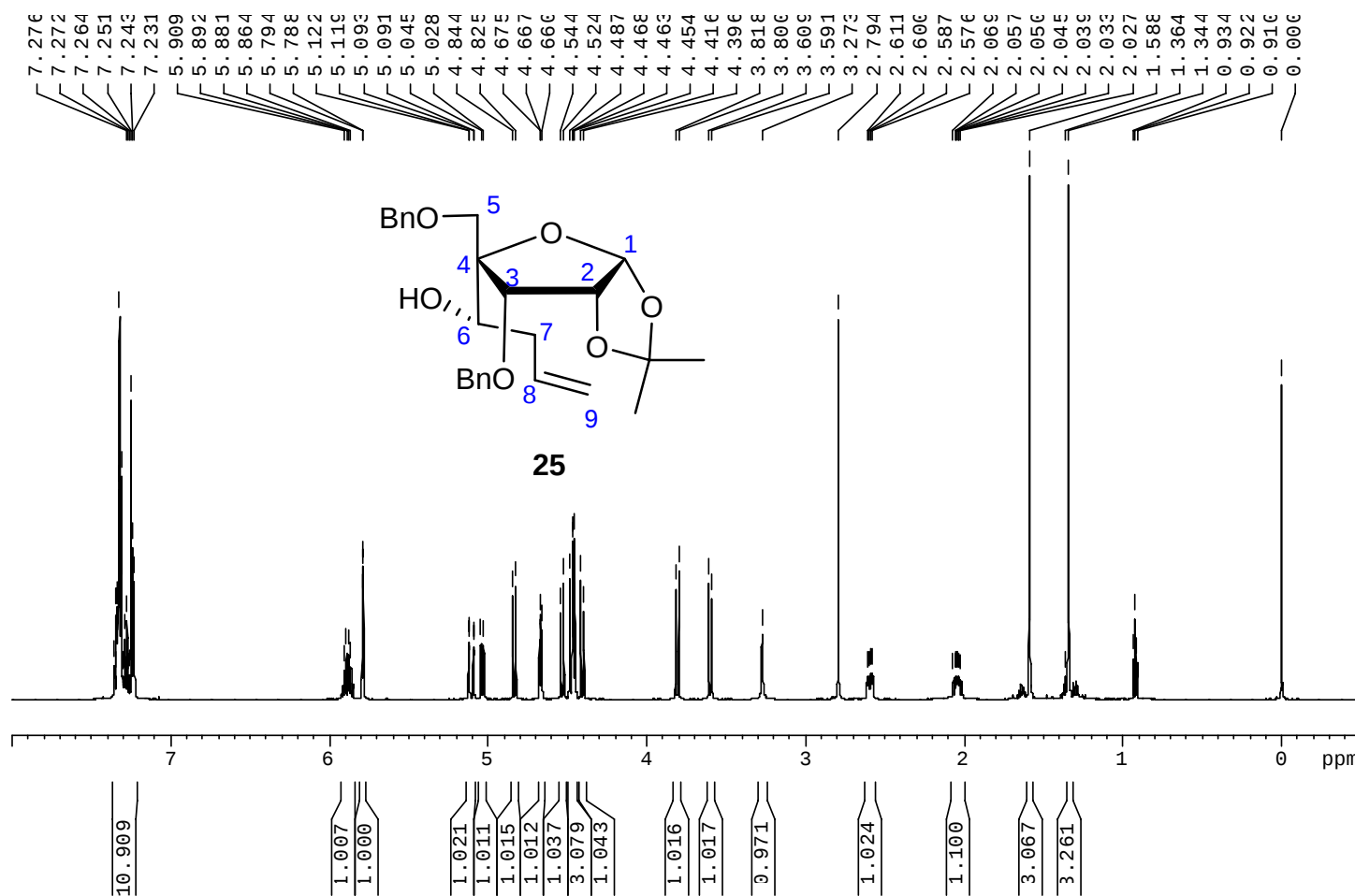


Figure SII.1. ^1H NMR spectrum of compound 25.

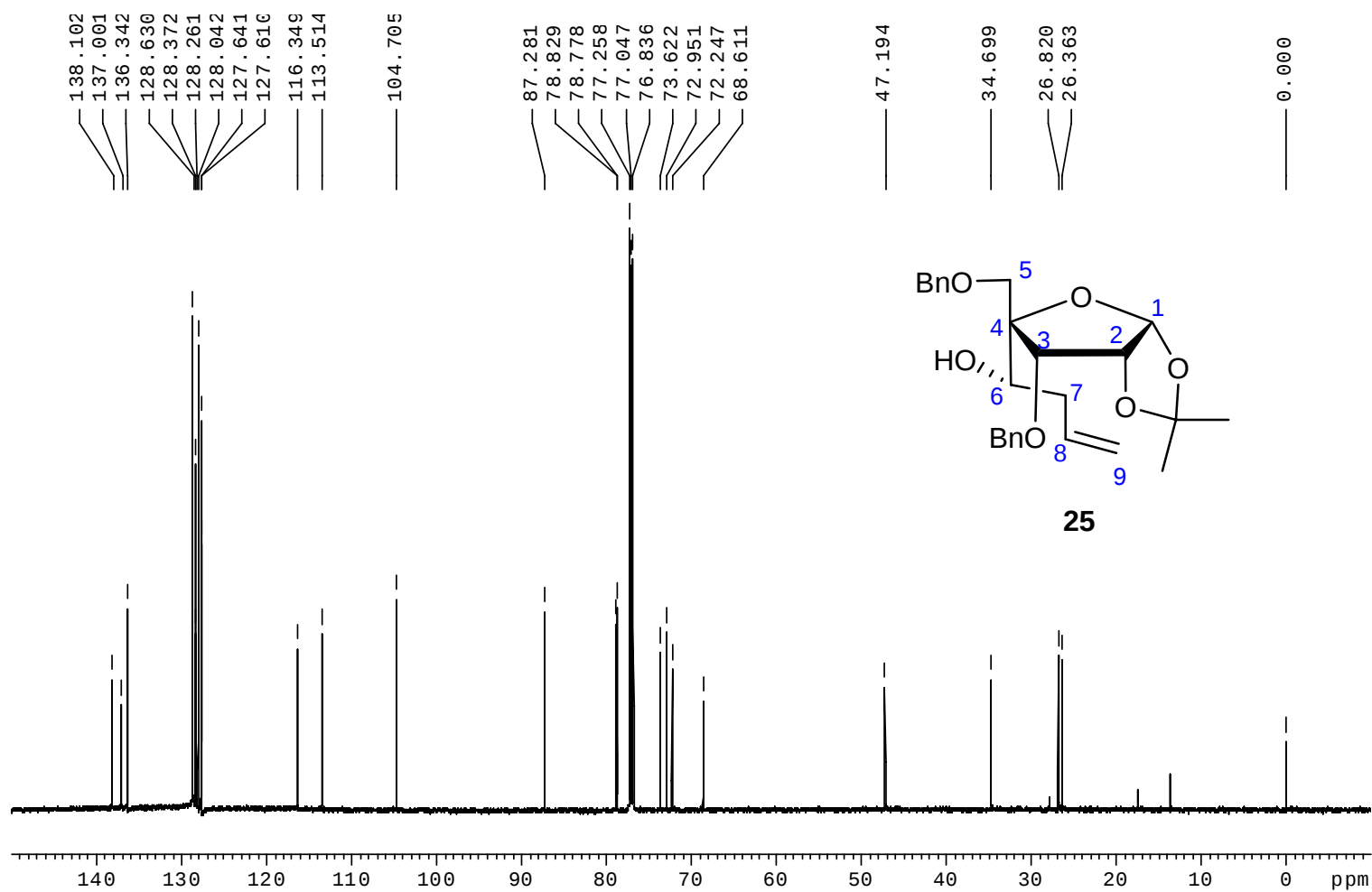


Figure SII.2. ^{13}C NMR spectrum of compound 25.

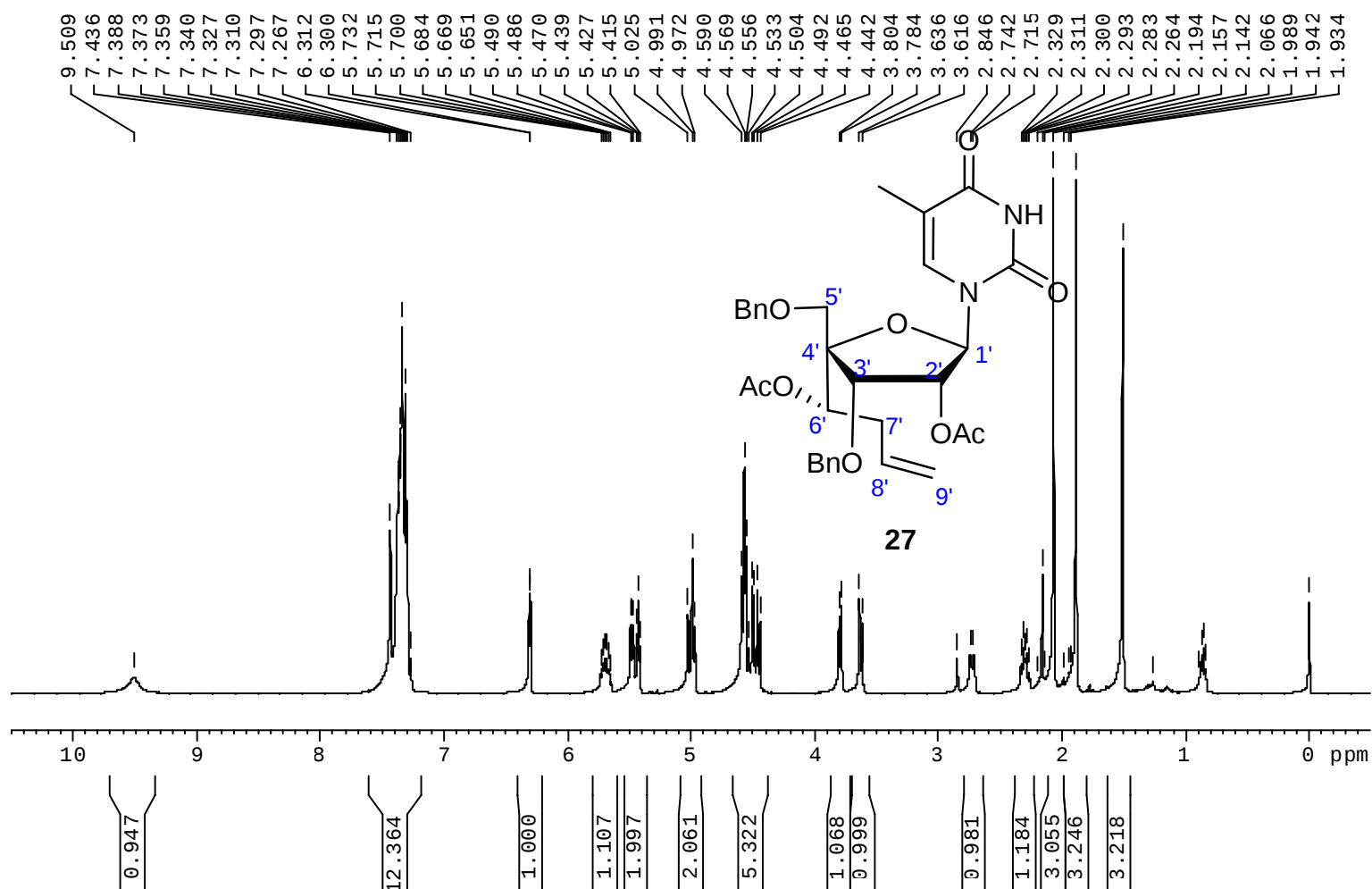


Figure SII.3. ^1H NMR spectrum of compound 27.

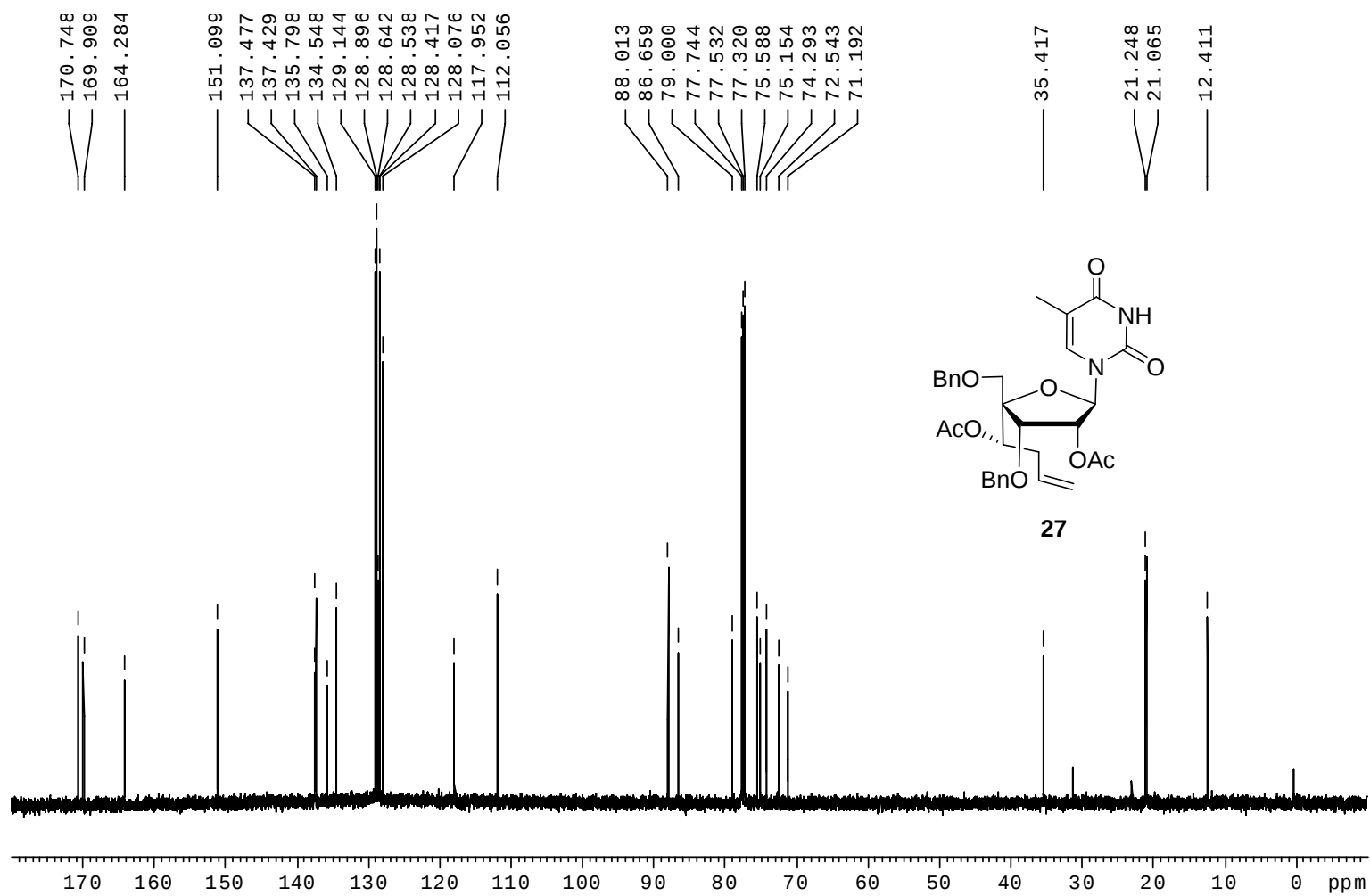


Figure SII.4. ^{13}C NMR spectrum of compound 27.

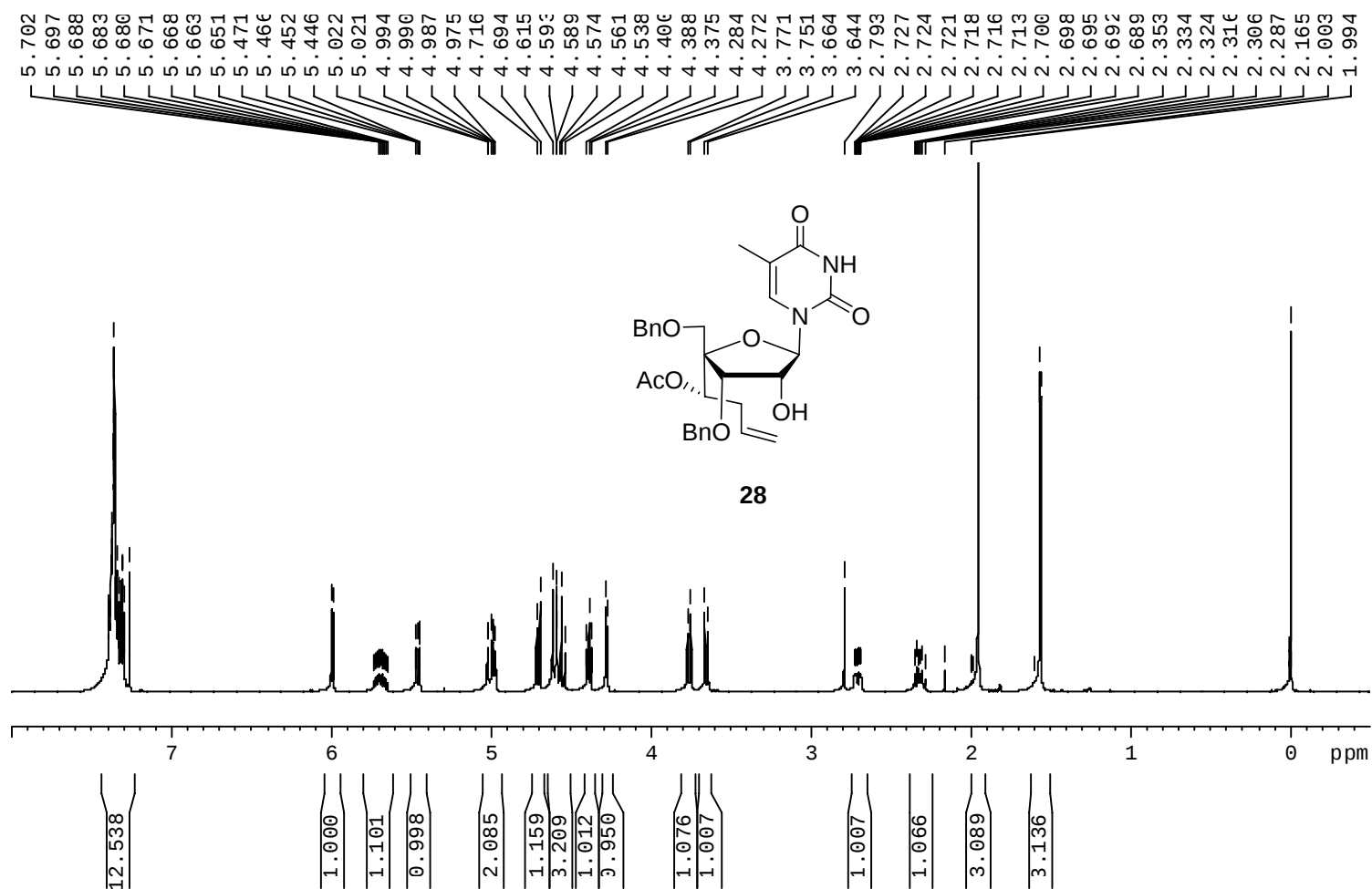


Figure SII.5. ^1H NMR spectrum of compound 28.

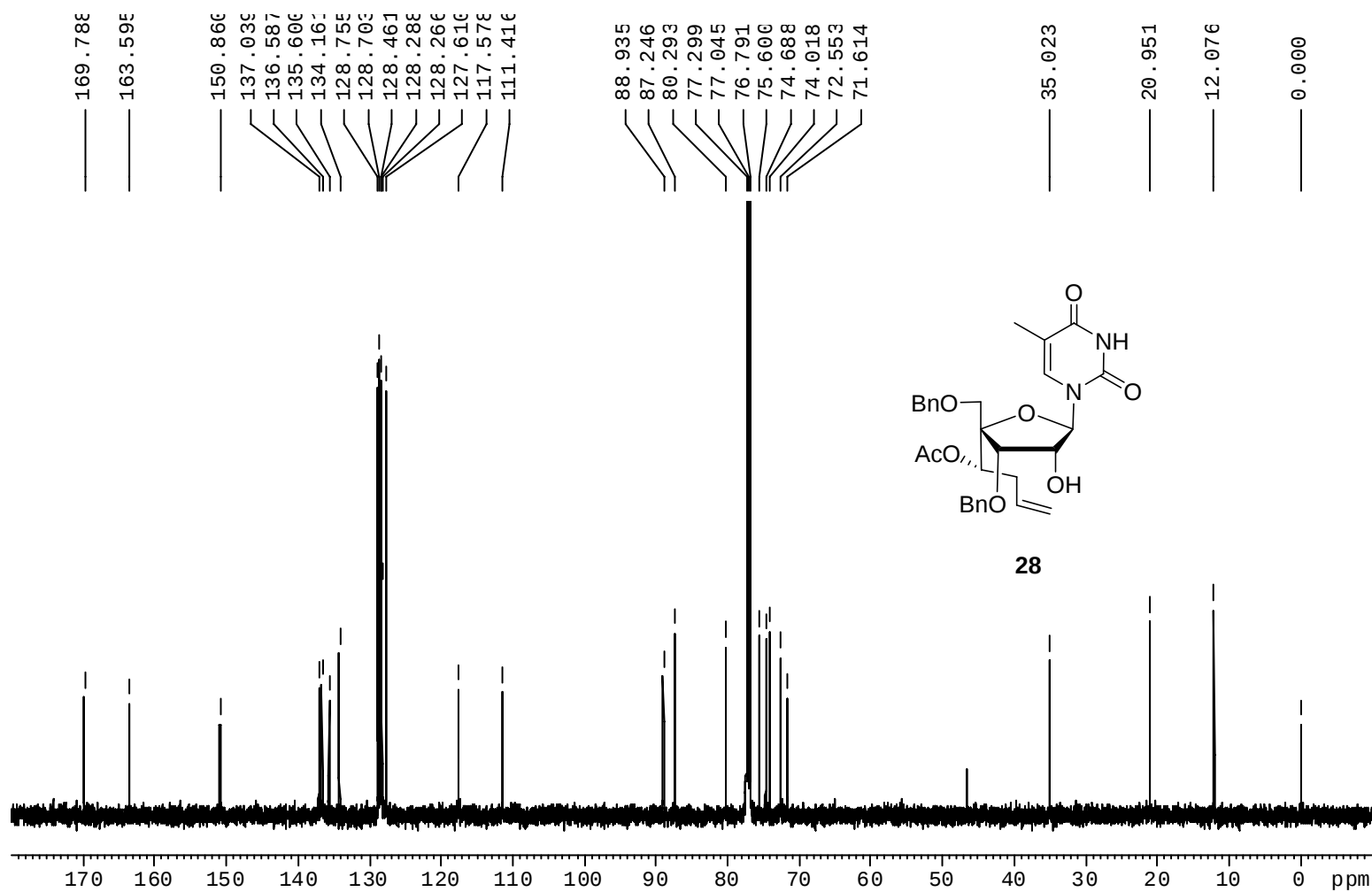


Figure SII.6. ^{13}C NMR spectrum of compound 28.

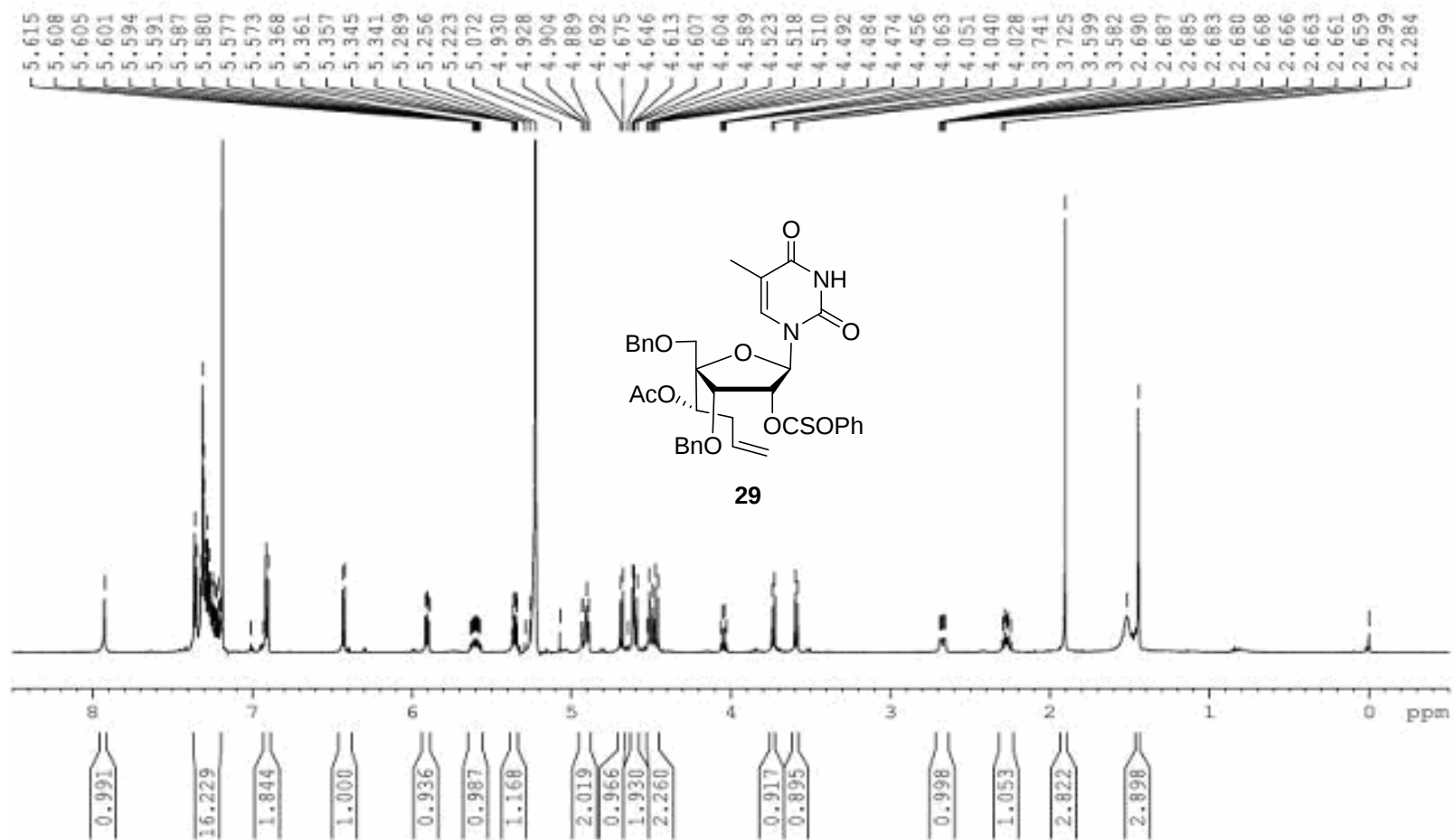


Figure SII.7. ^1H NMR spectrum of compound 29.

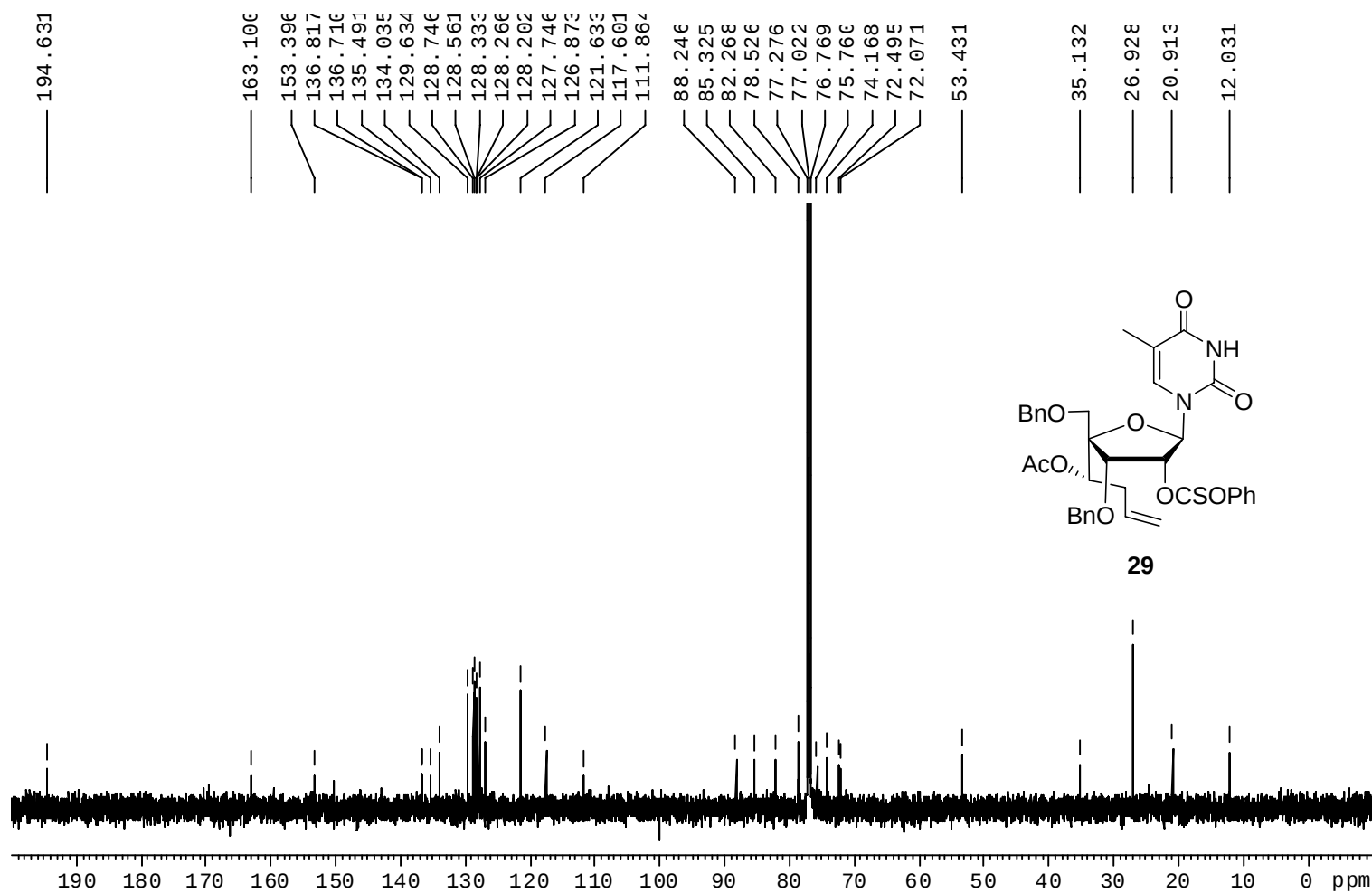


Figure SII.8. ^{13}C NMR spectrum of compound 29.

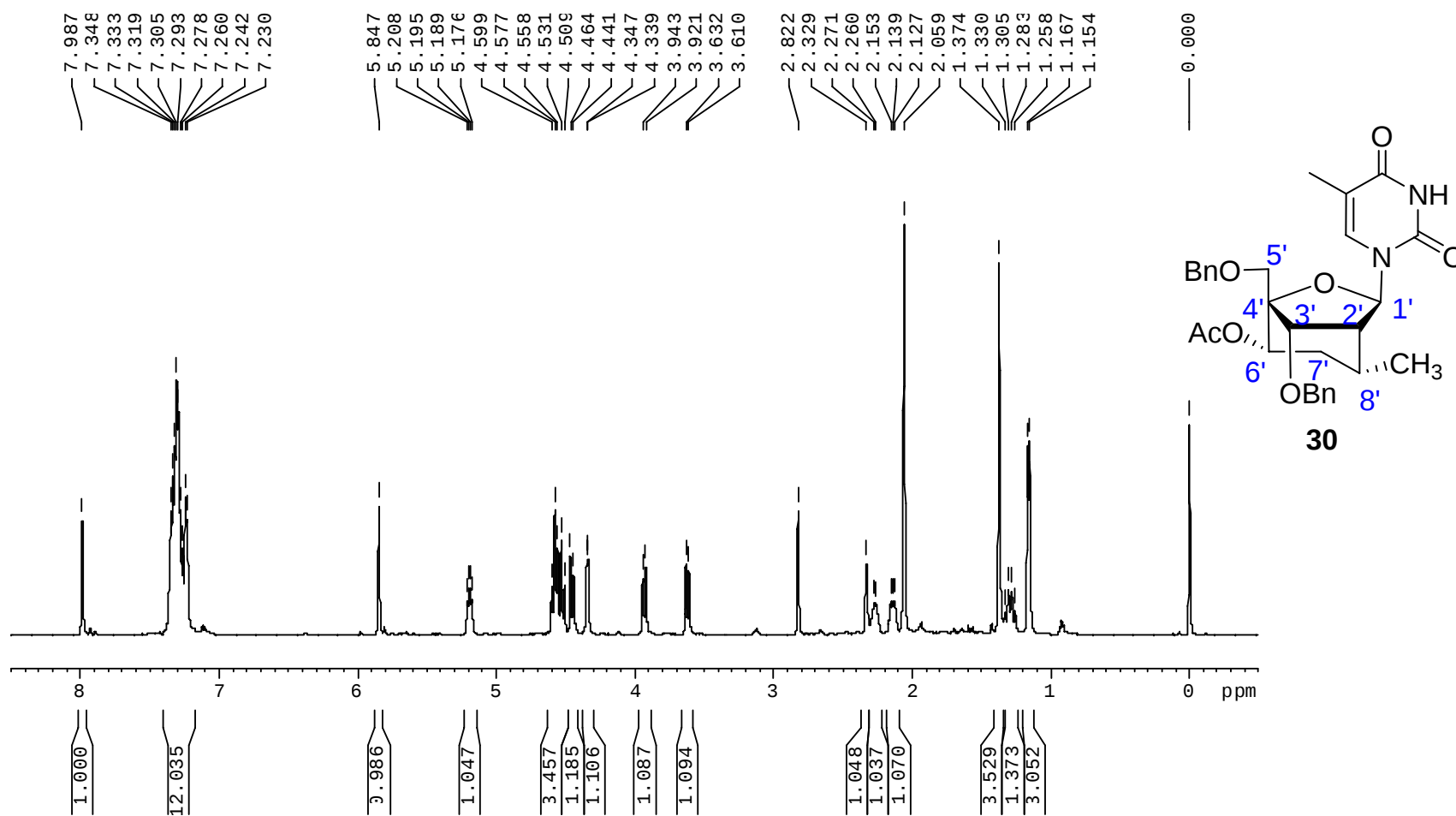


Figure SII.9. ¹H NMR spectrum of compound 30.

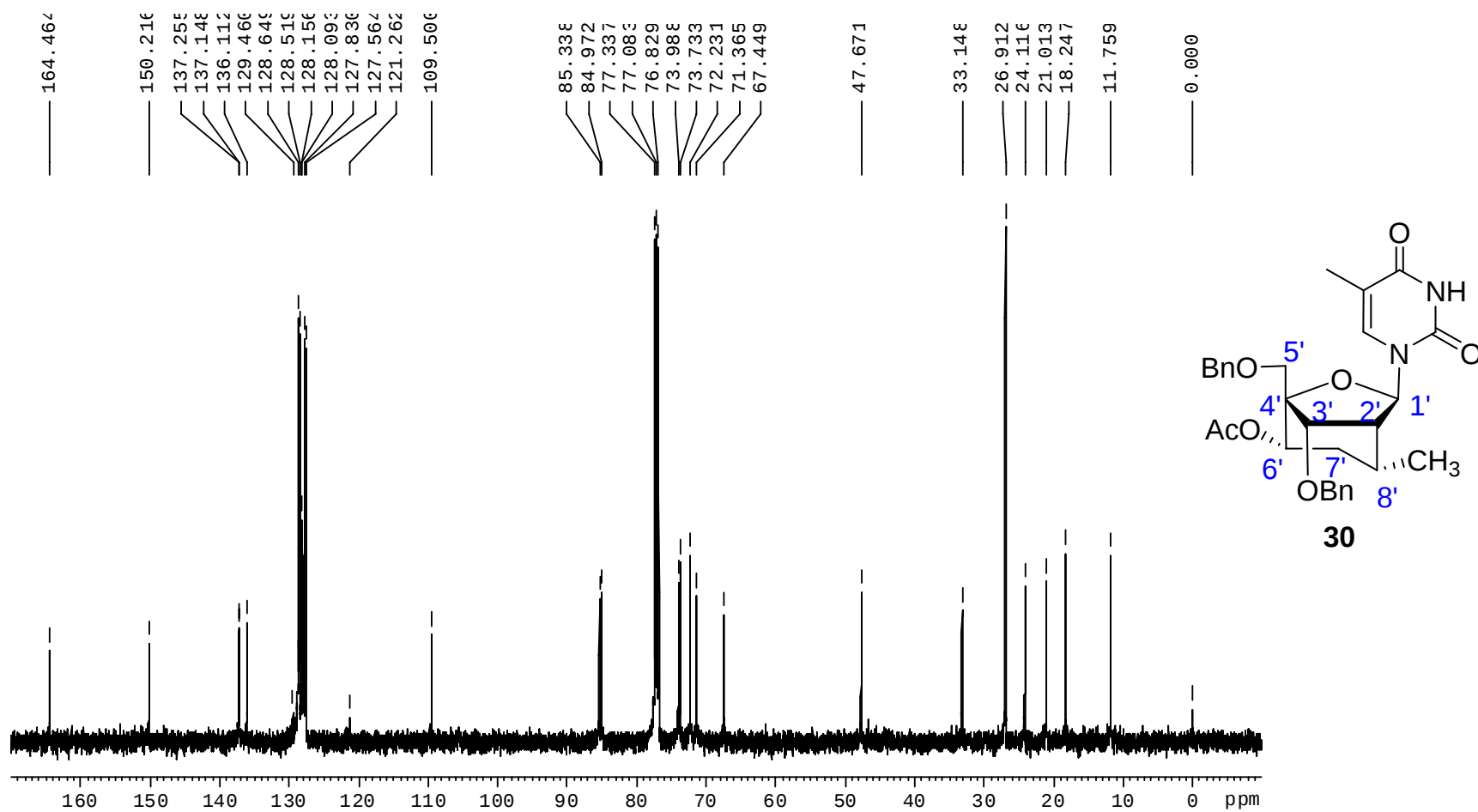
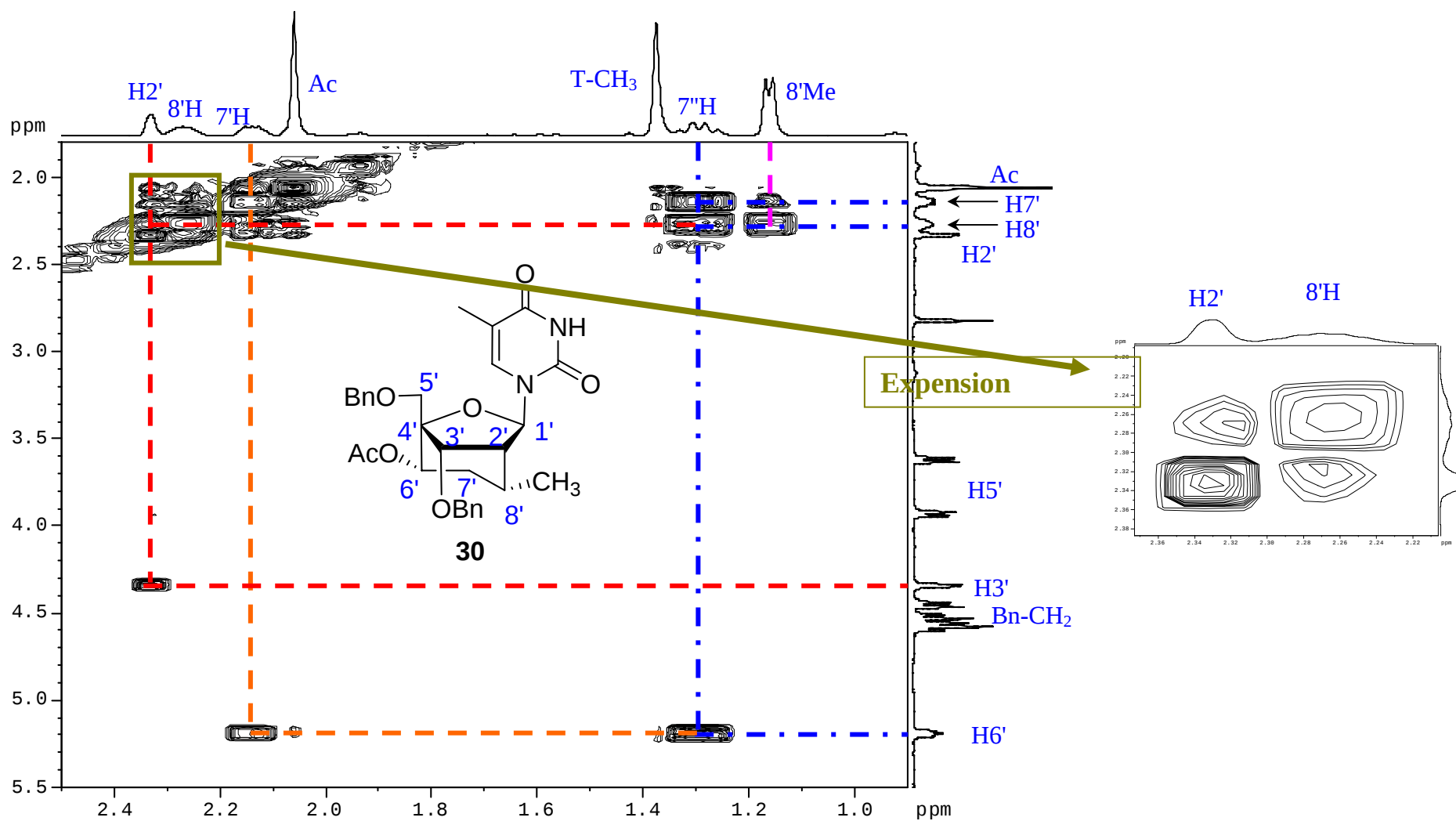


Figure SII.10. ^{13}C NMR spectrum of compound 30.



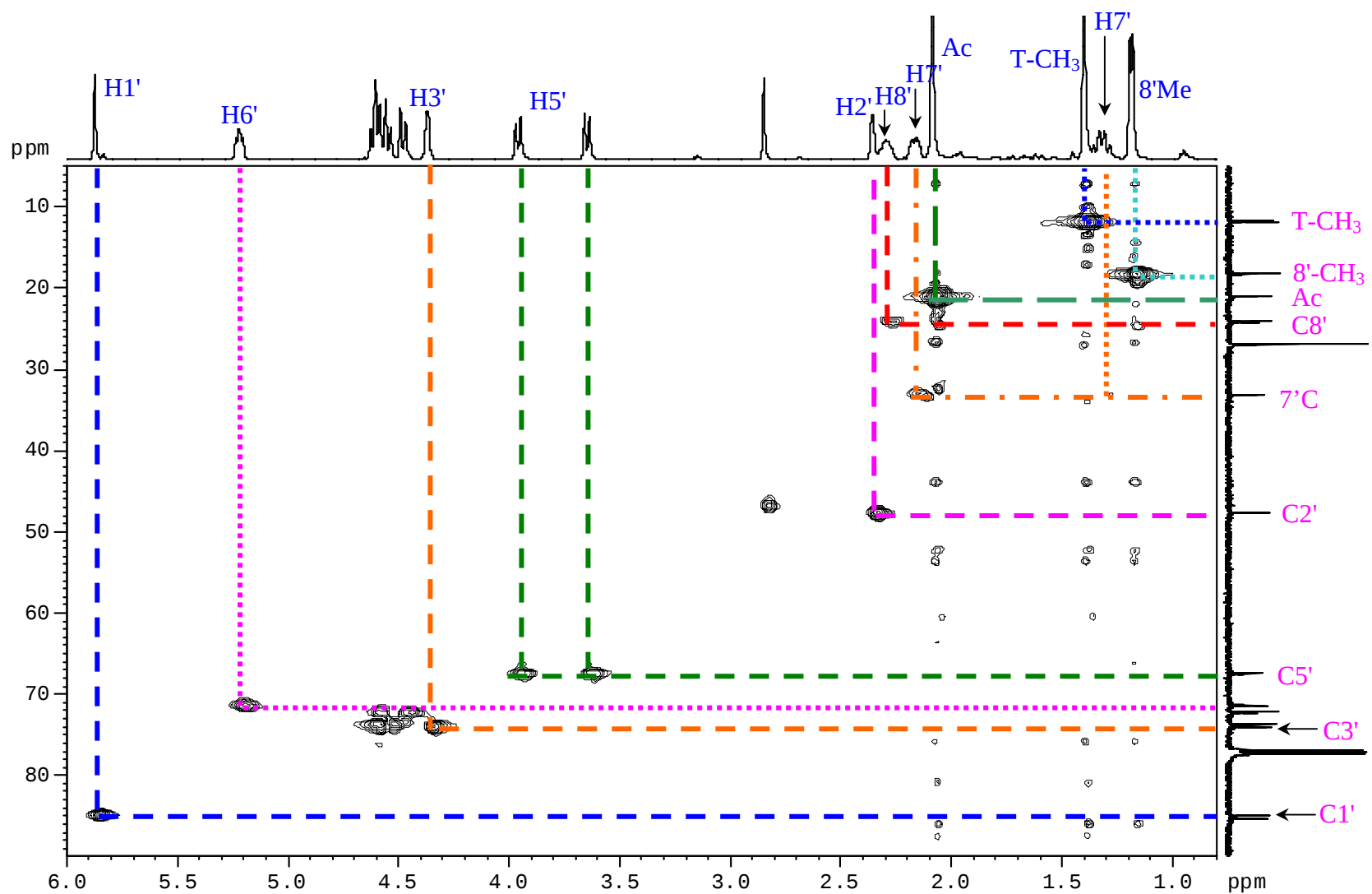
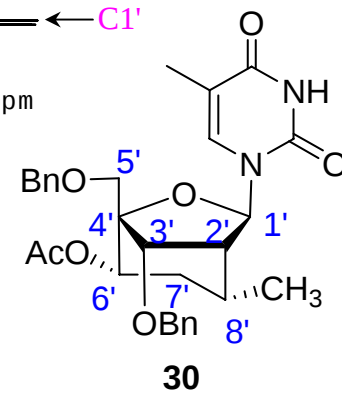


Figure SII.12. HMQC spectrum of compound 30.



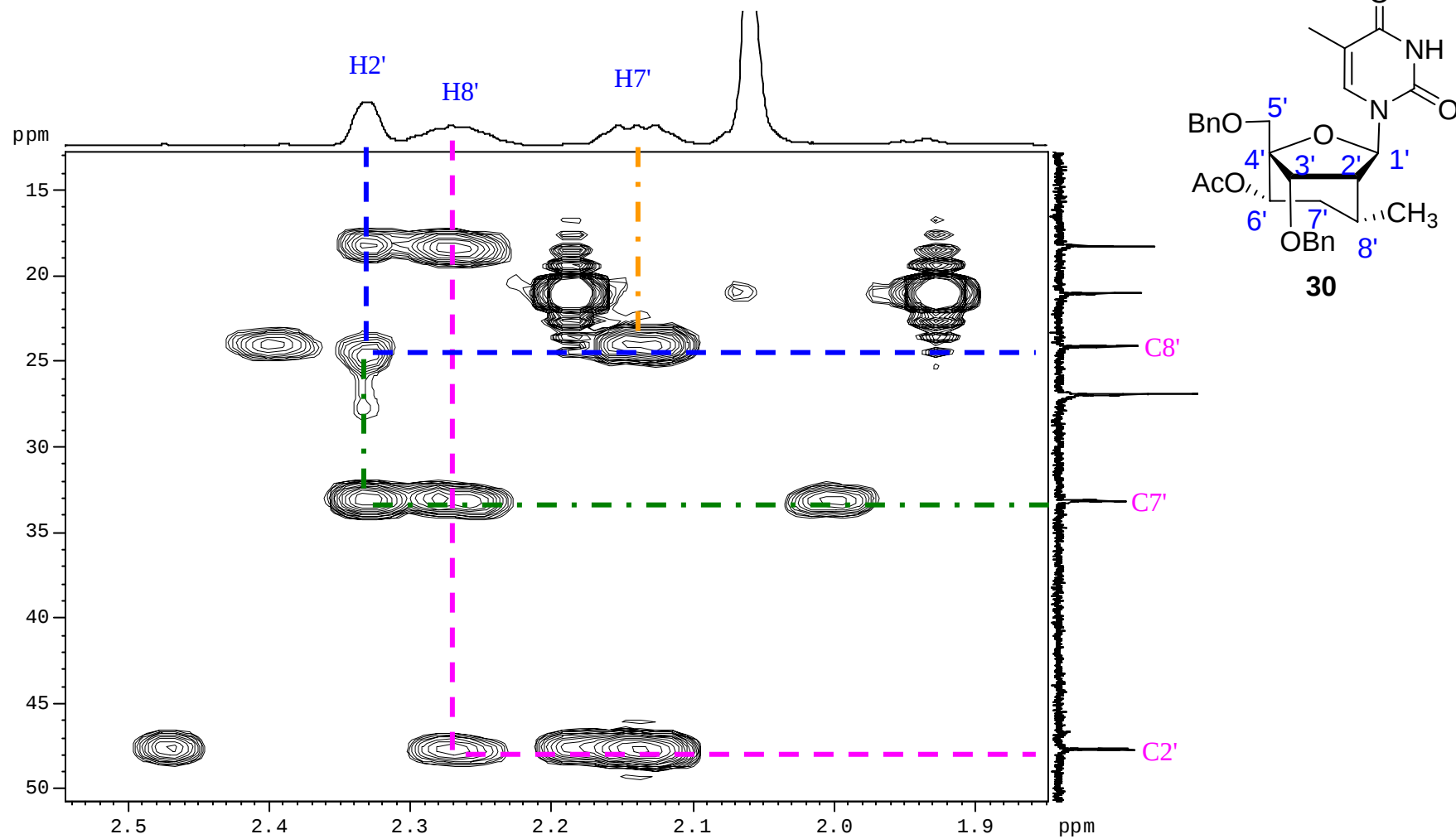


Figure SII.13. HMBC spectrum of compound 30.

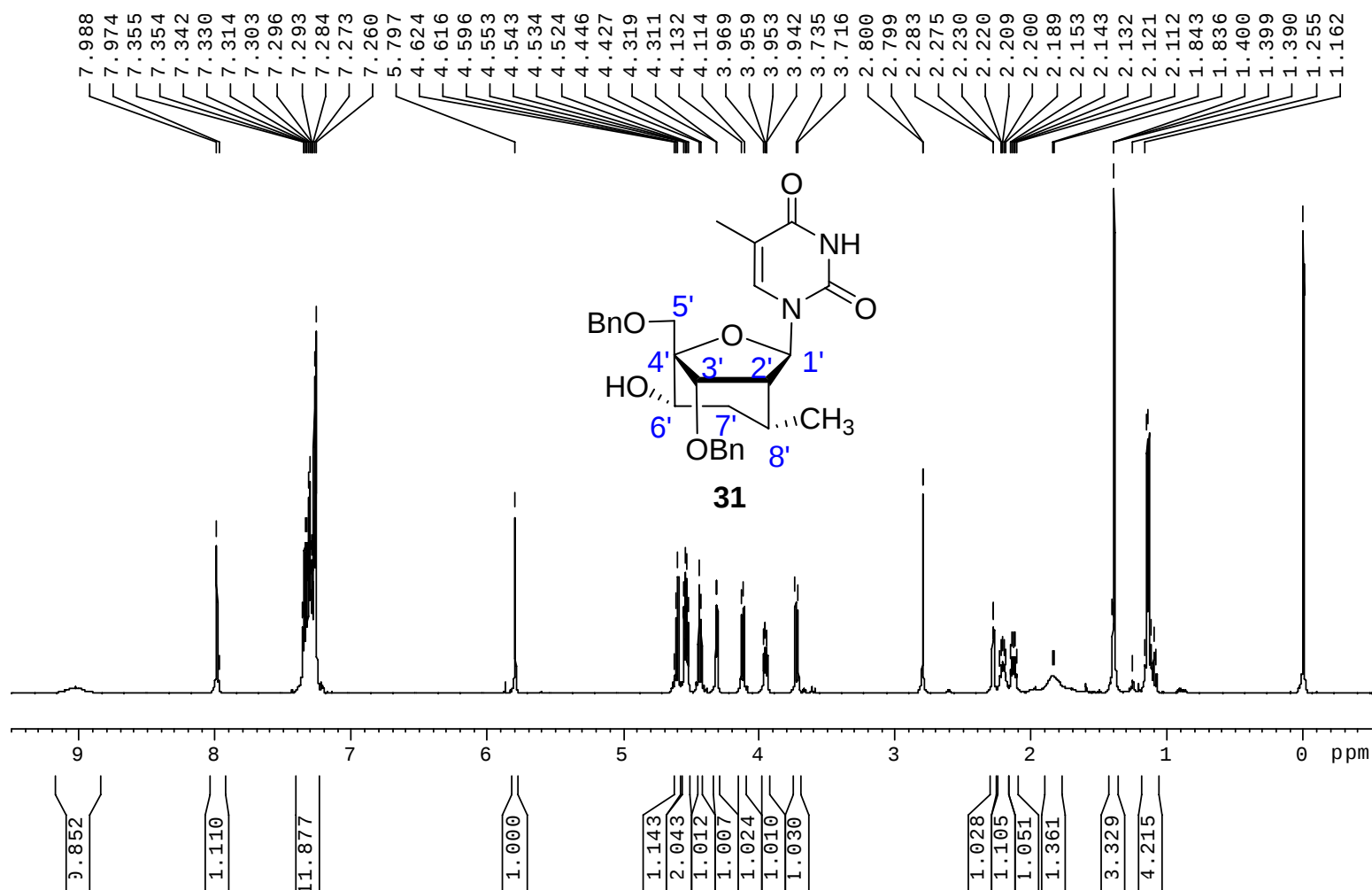


Figure SII.14. ¹H NMR spectrum of compound 31.

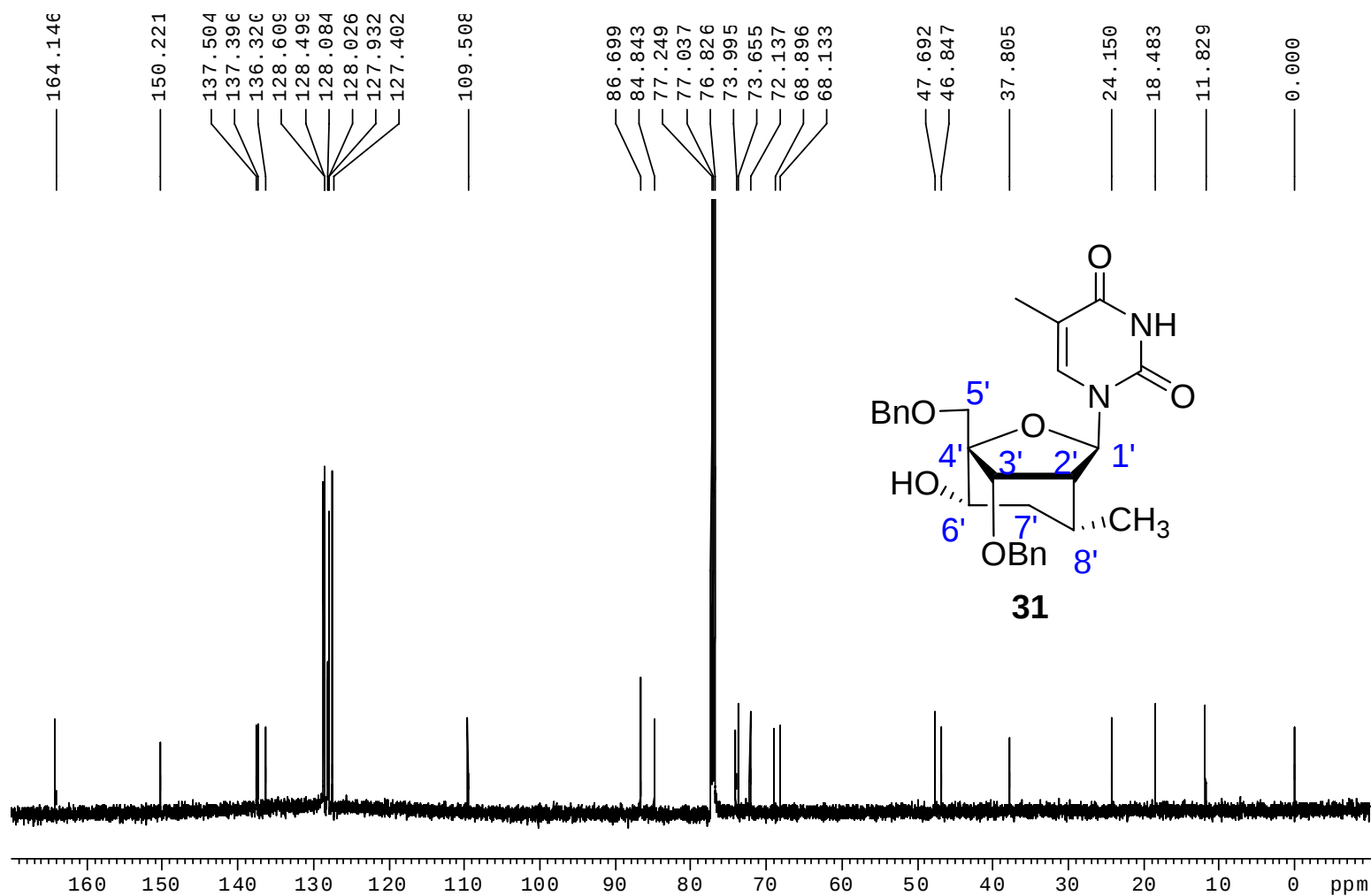


Figure SII.15. ¹³C NMR spectrum of compound 31.

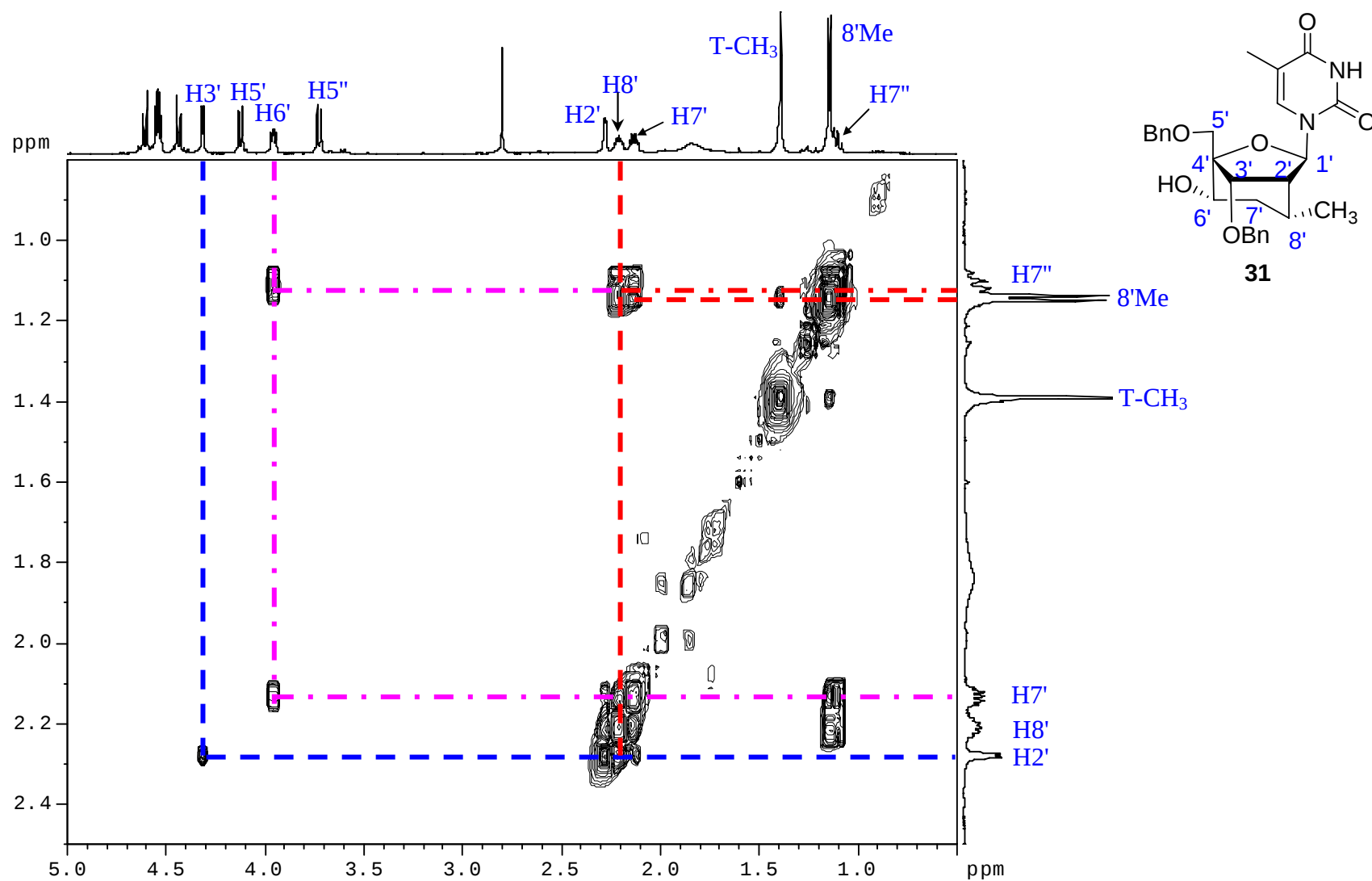


Figure SII.16. COSY spectrum of compound 31.

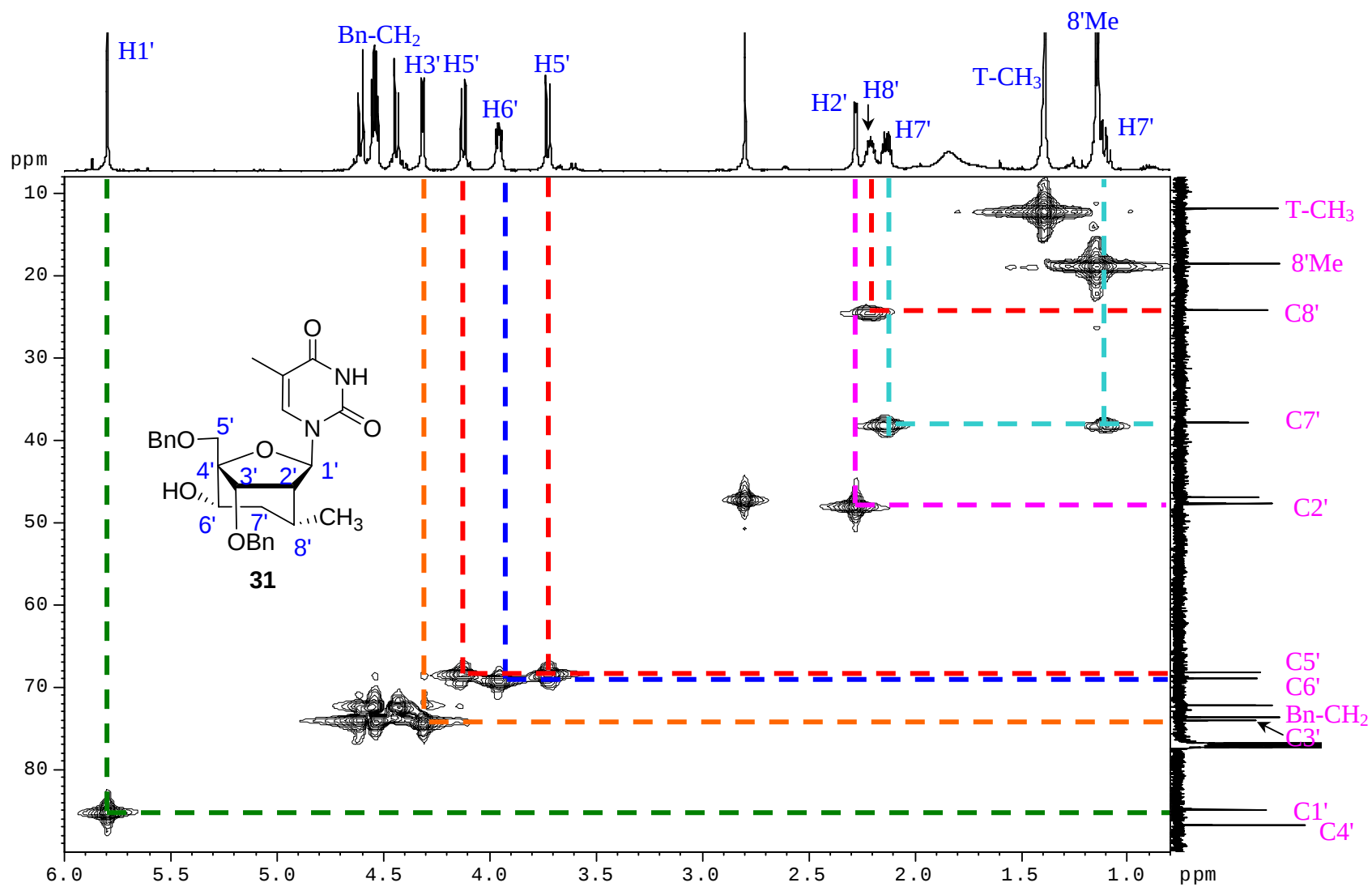


Figure SII.17. HMBC spectrum of compound 31.

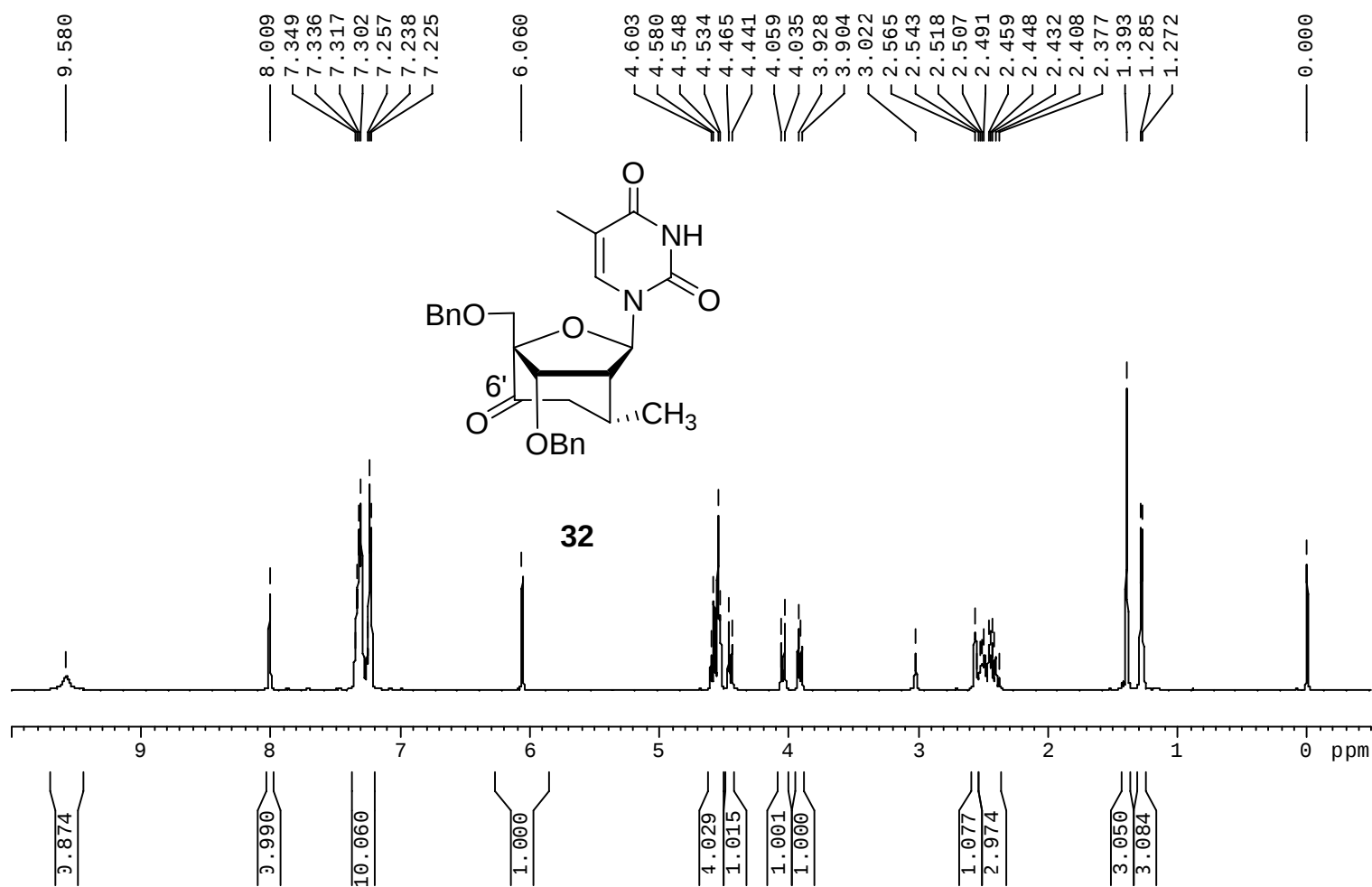


Figure SII.18. ¹H NMR spectrum of compound 32.

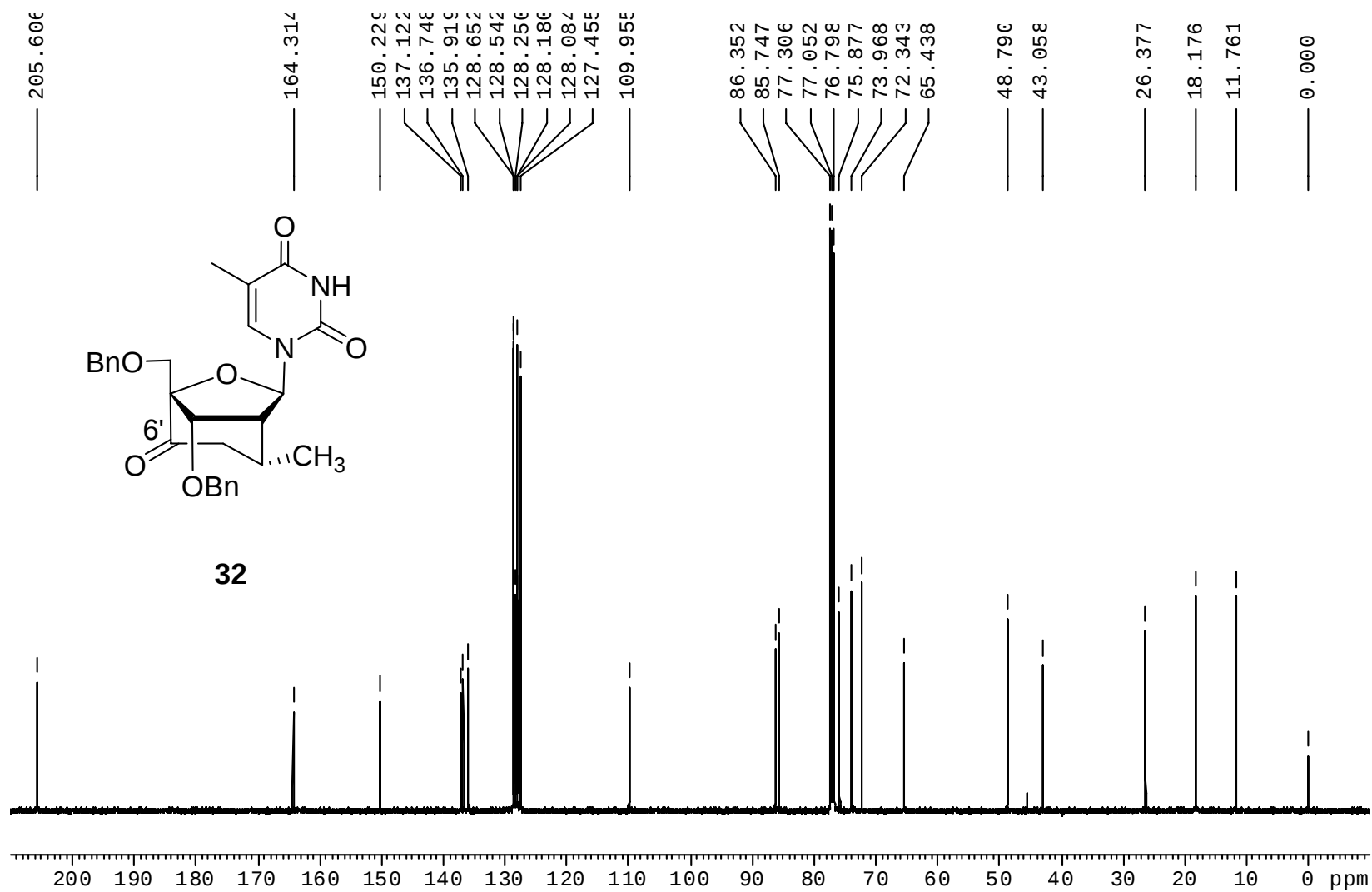


Figure SII.19. ^{13}C NMR spectrum of compound 32.

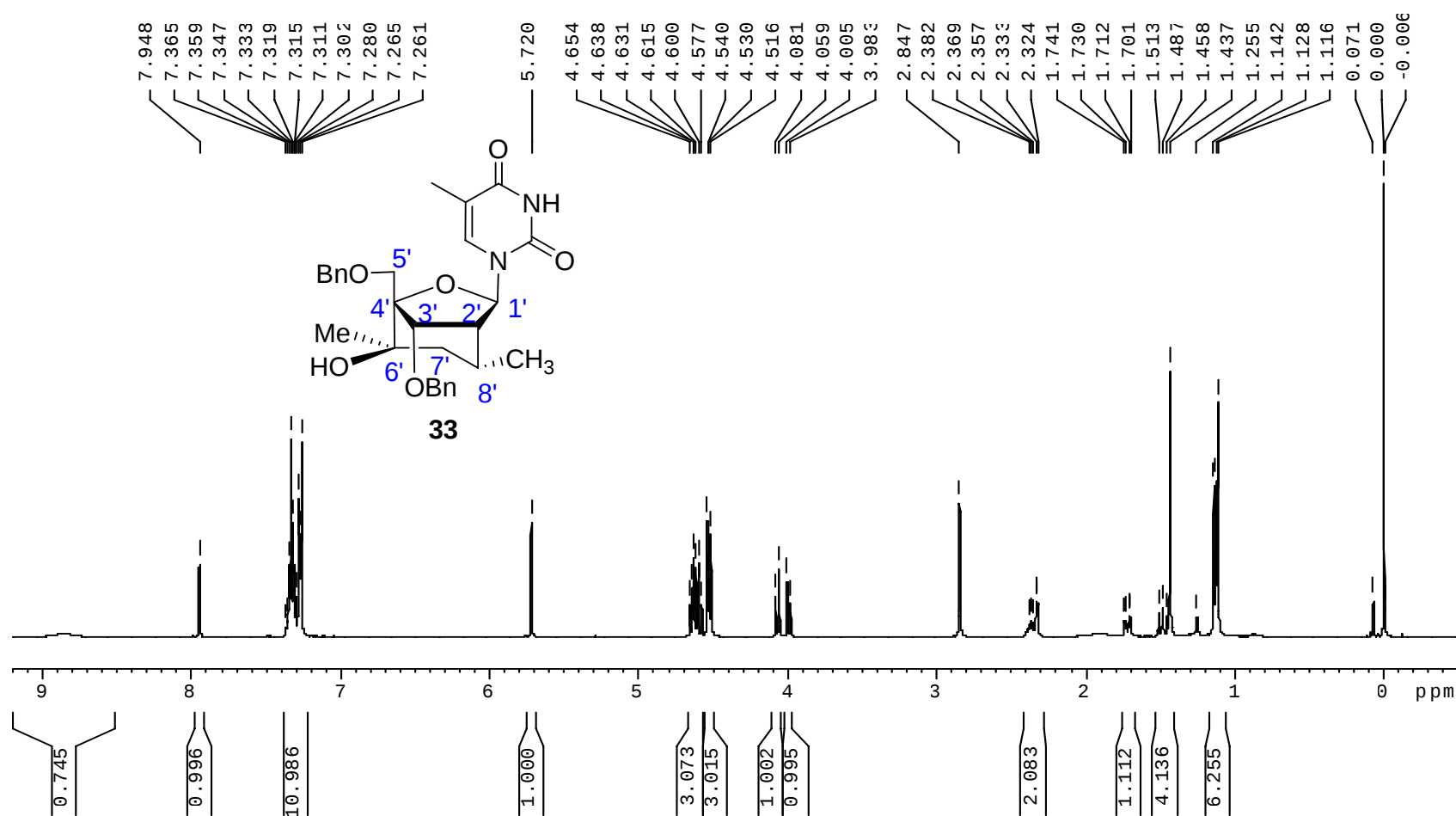


Figure SII.20. ^1H NMR spectrum of compound 33.

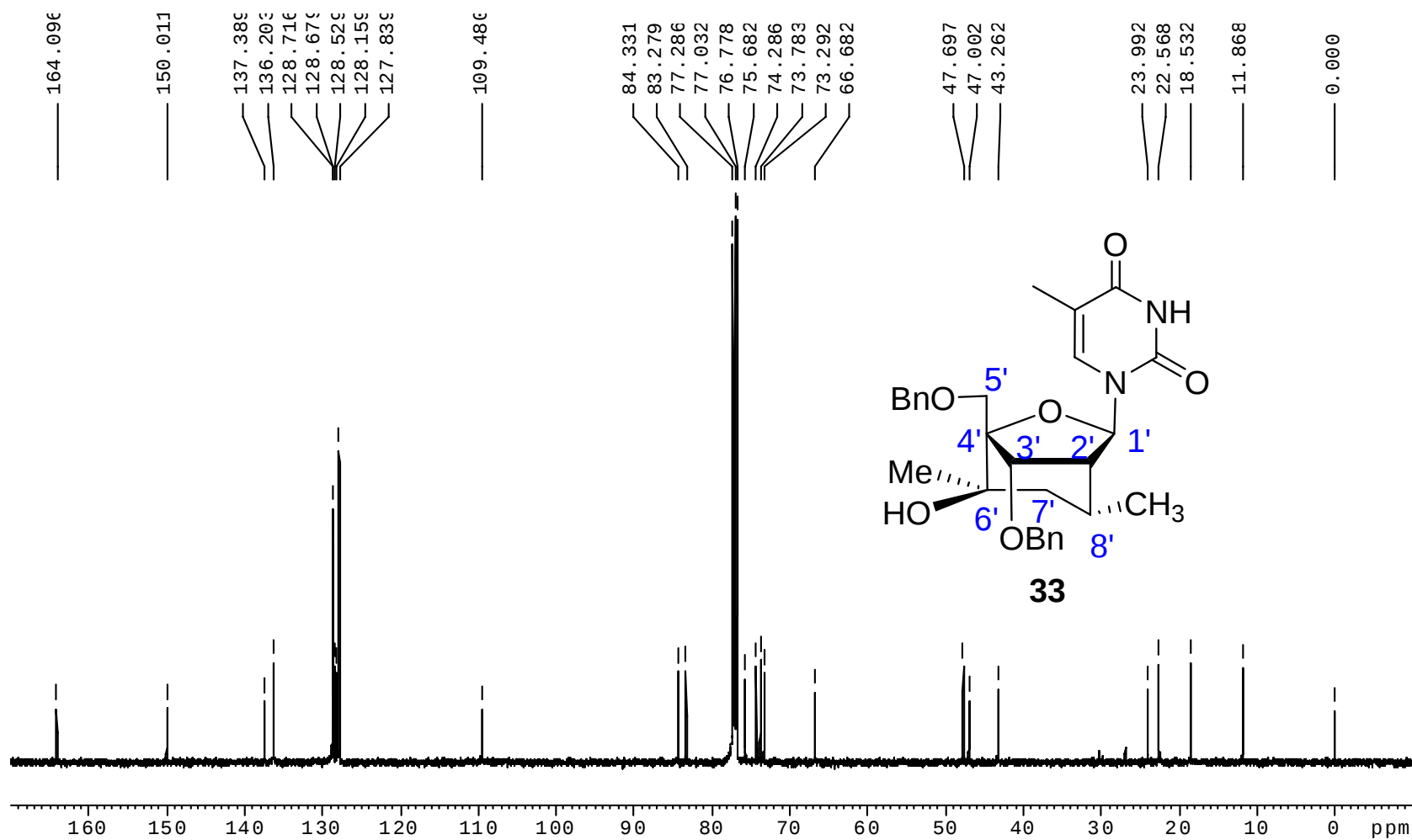


Figure SII.21. ¹³C NMR spectrum of compound 33.

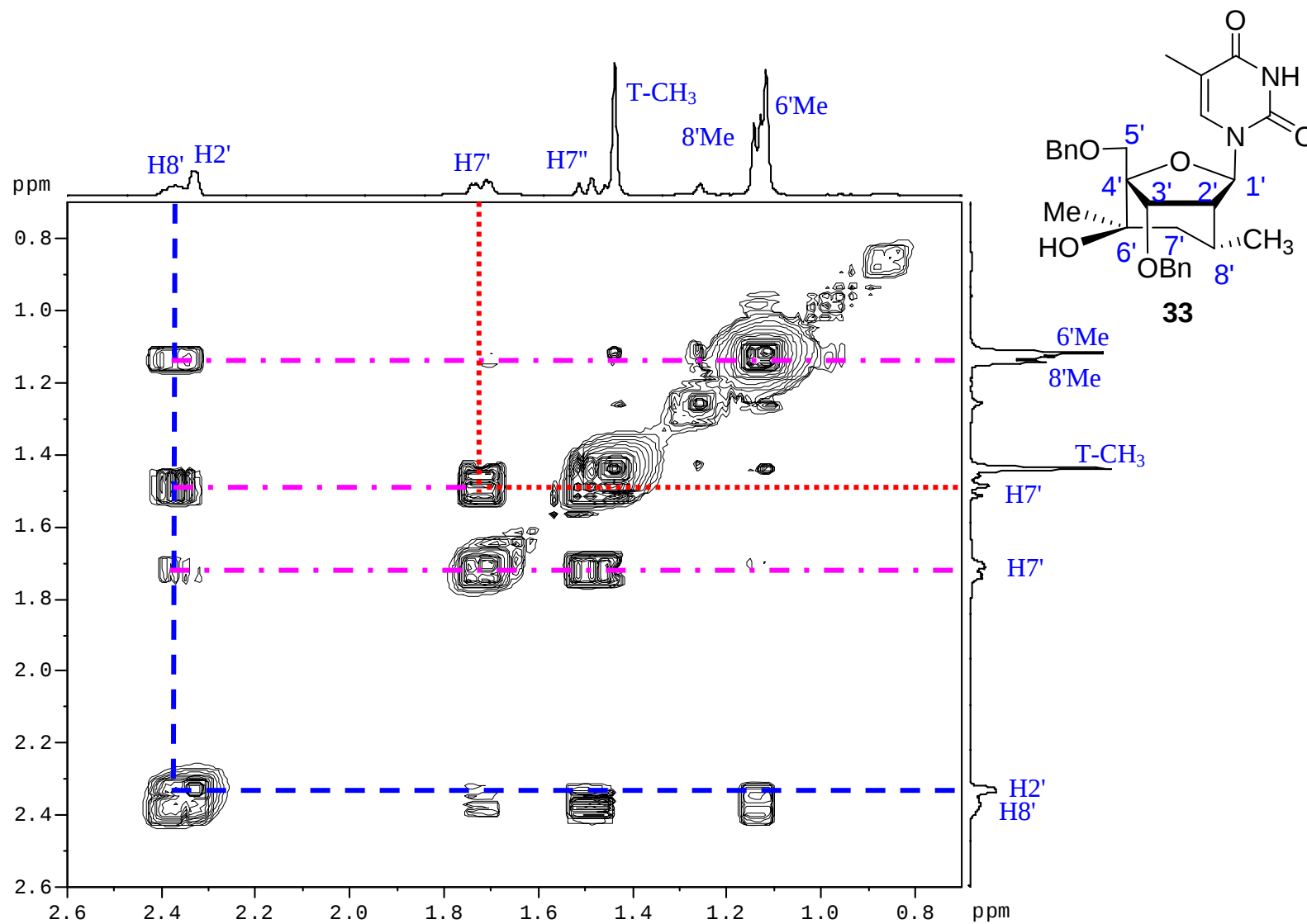


Figure SII.22. COSY spectrum of compound 33.

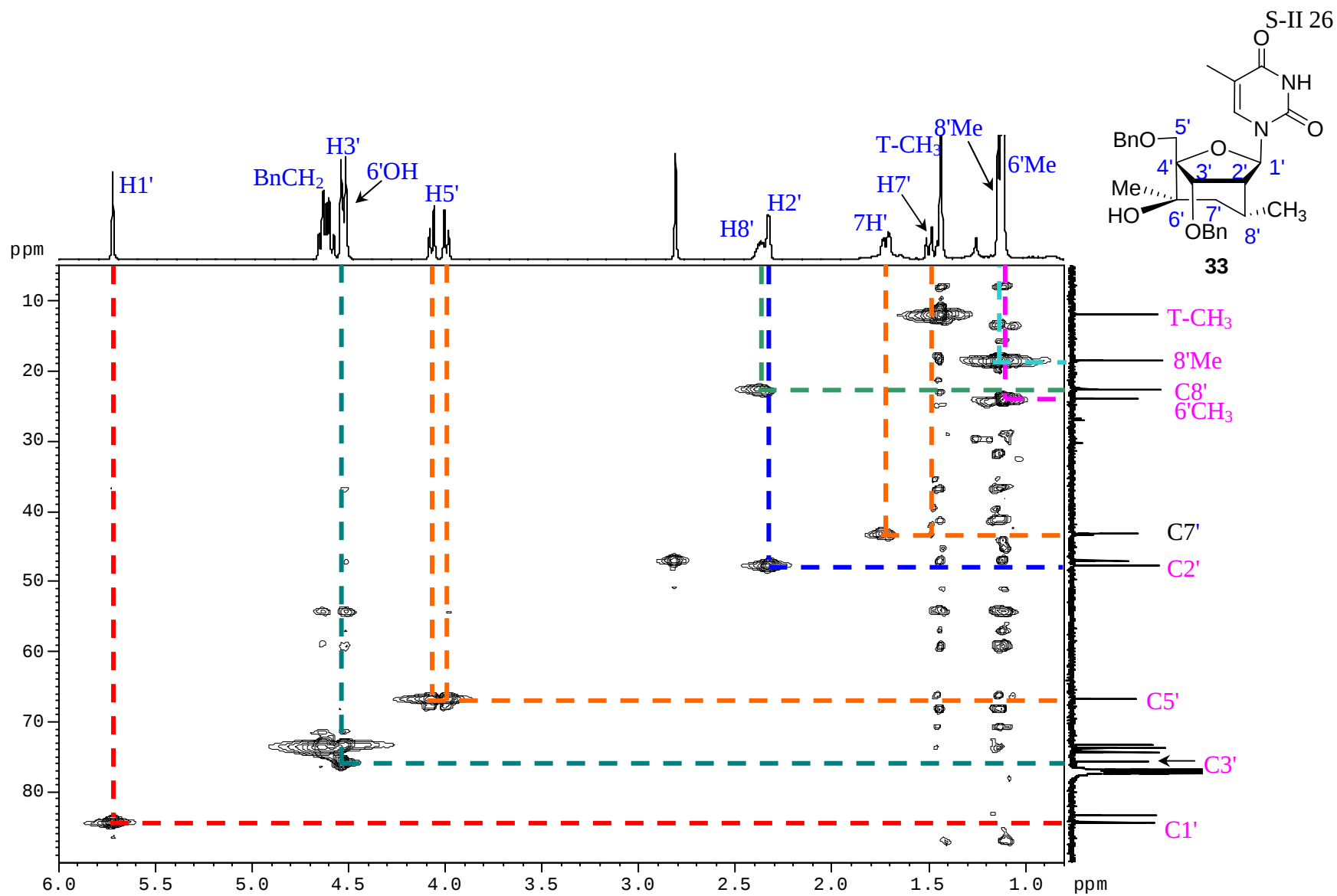


Figure SII.23. HMQC spectrum of compound 33.

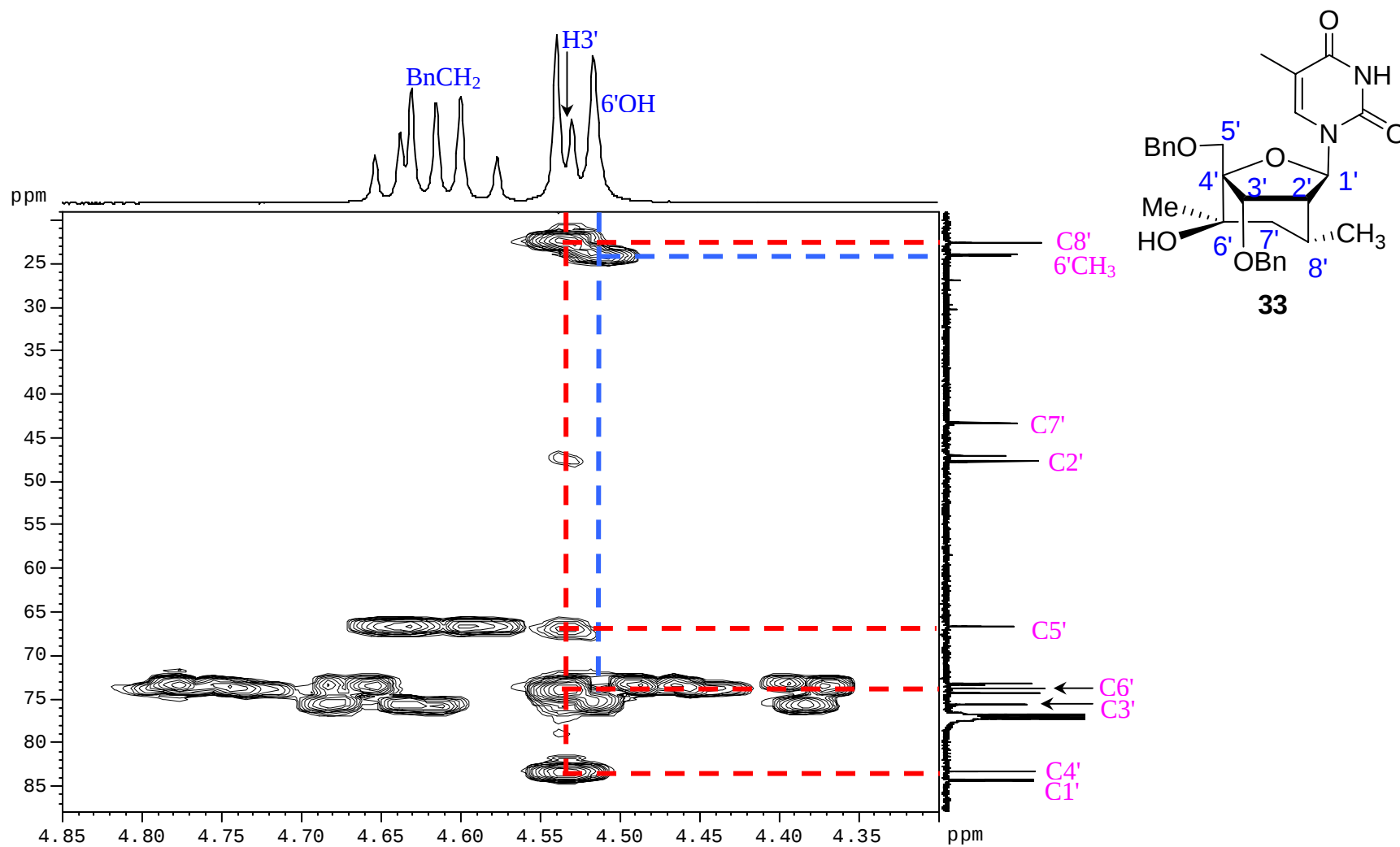


Figure SII.24. HMBC spectrum of compound 33.

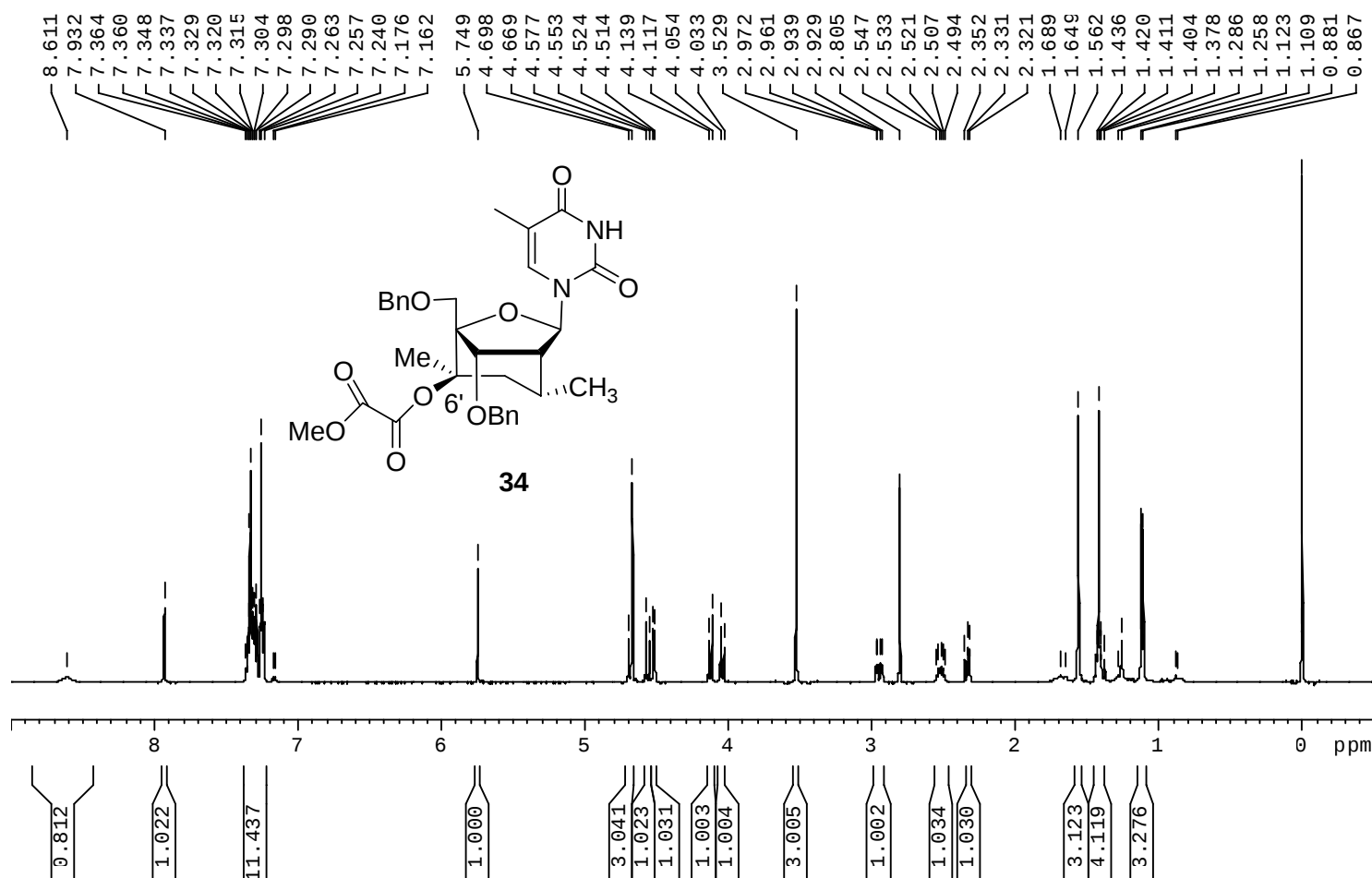


Figure SII.25. ^1H NMR spectrum of compound 34.

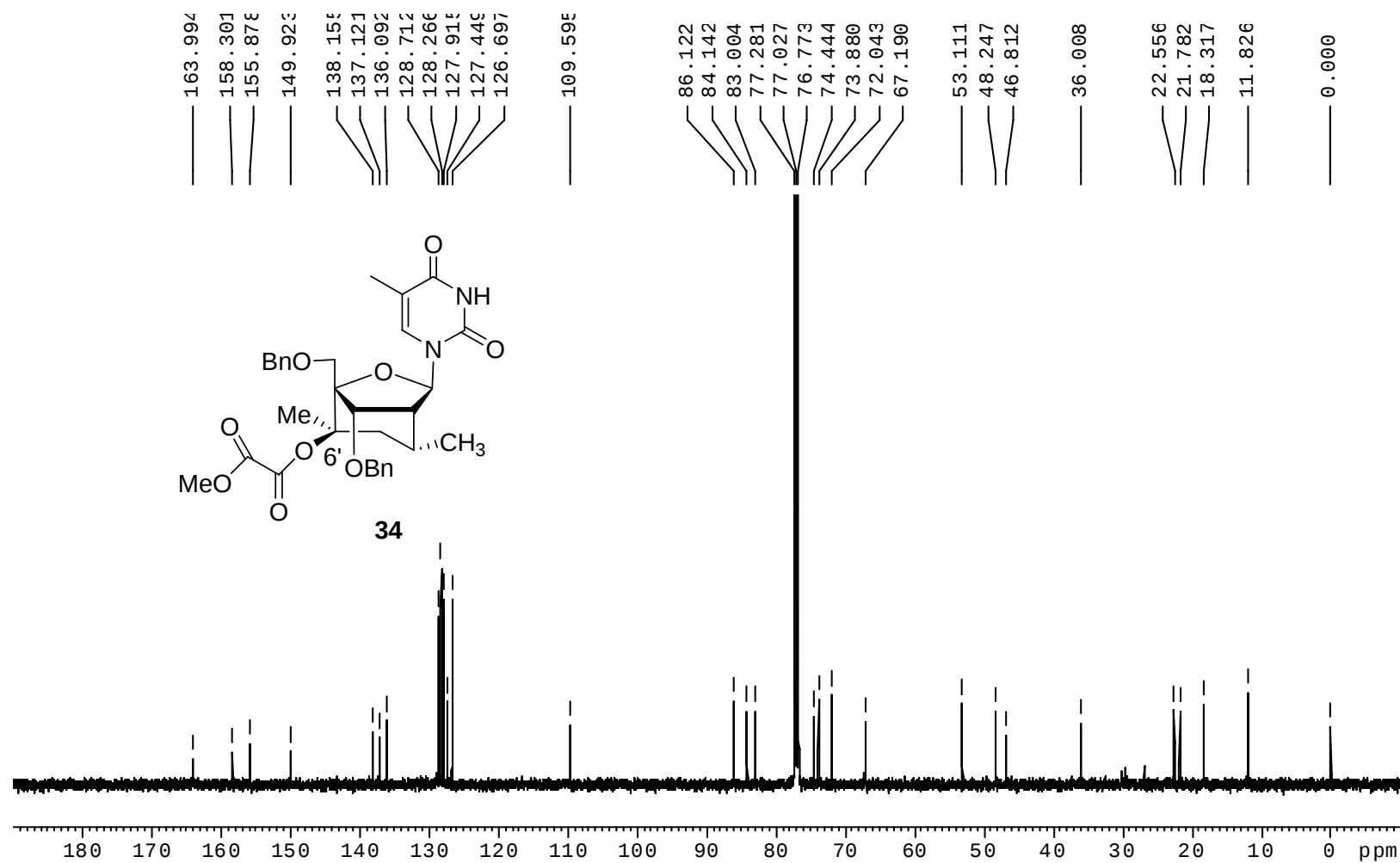


Figure SII.26. ^{13}C NMR spectrum of compound 34.

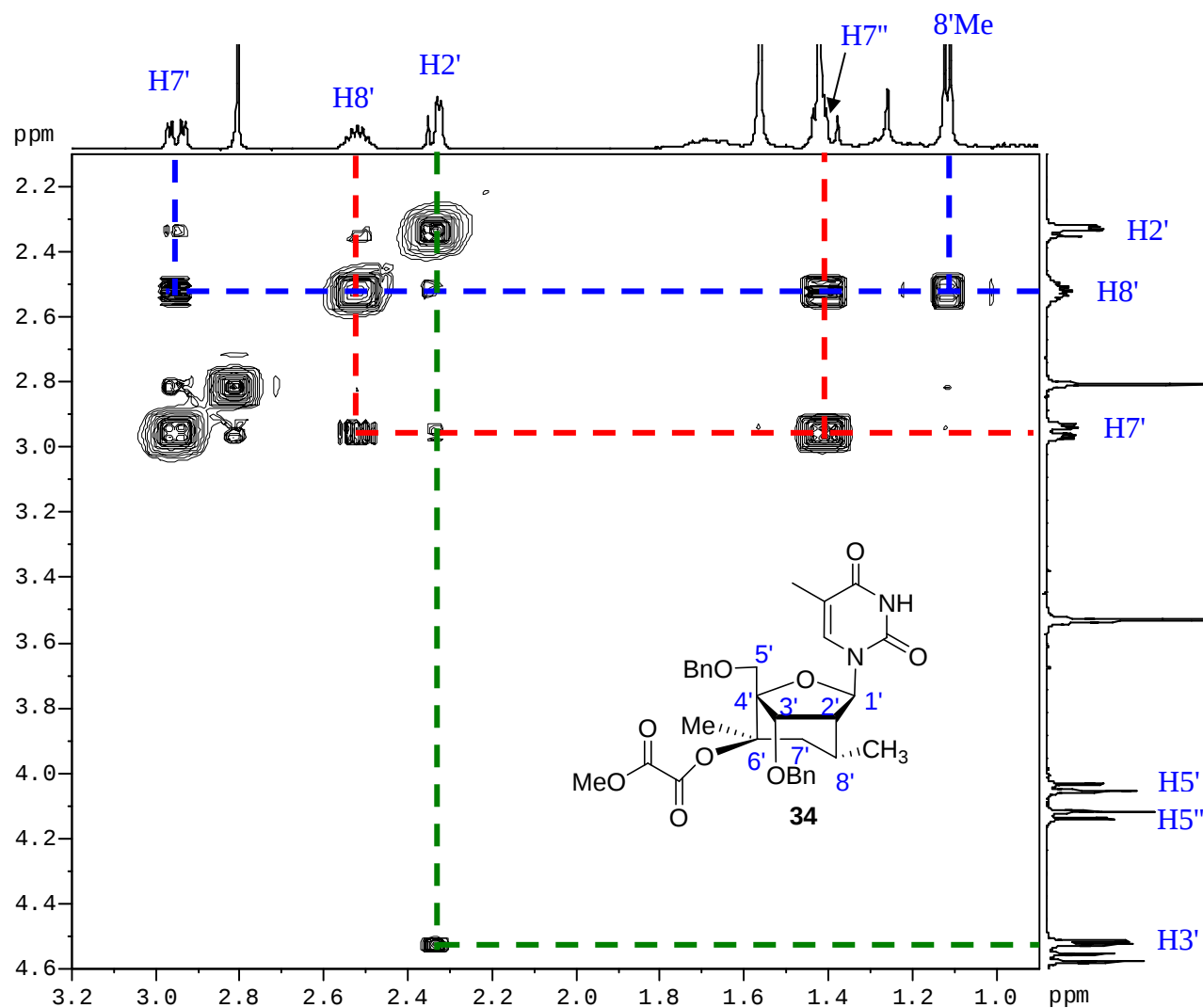


Figure SII.27. COSY spectrum of compound 34.

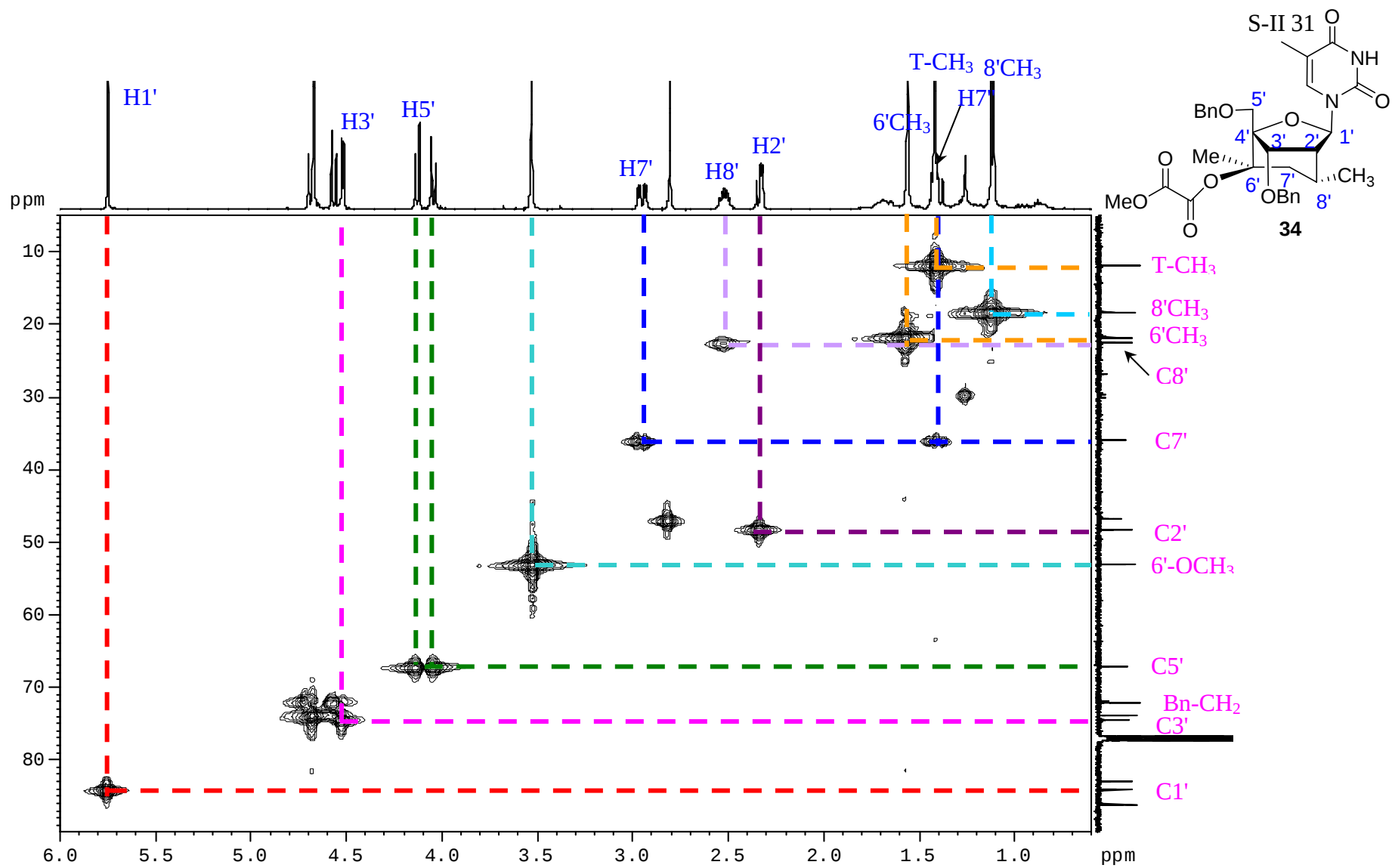


Figure SII.28. HMQC spectrum of compound 34.

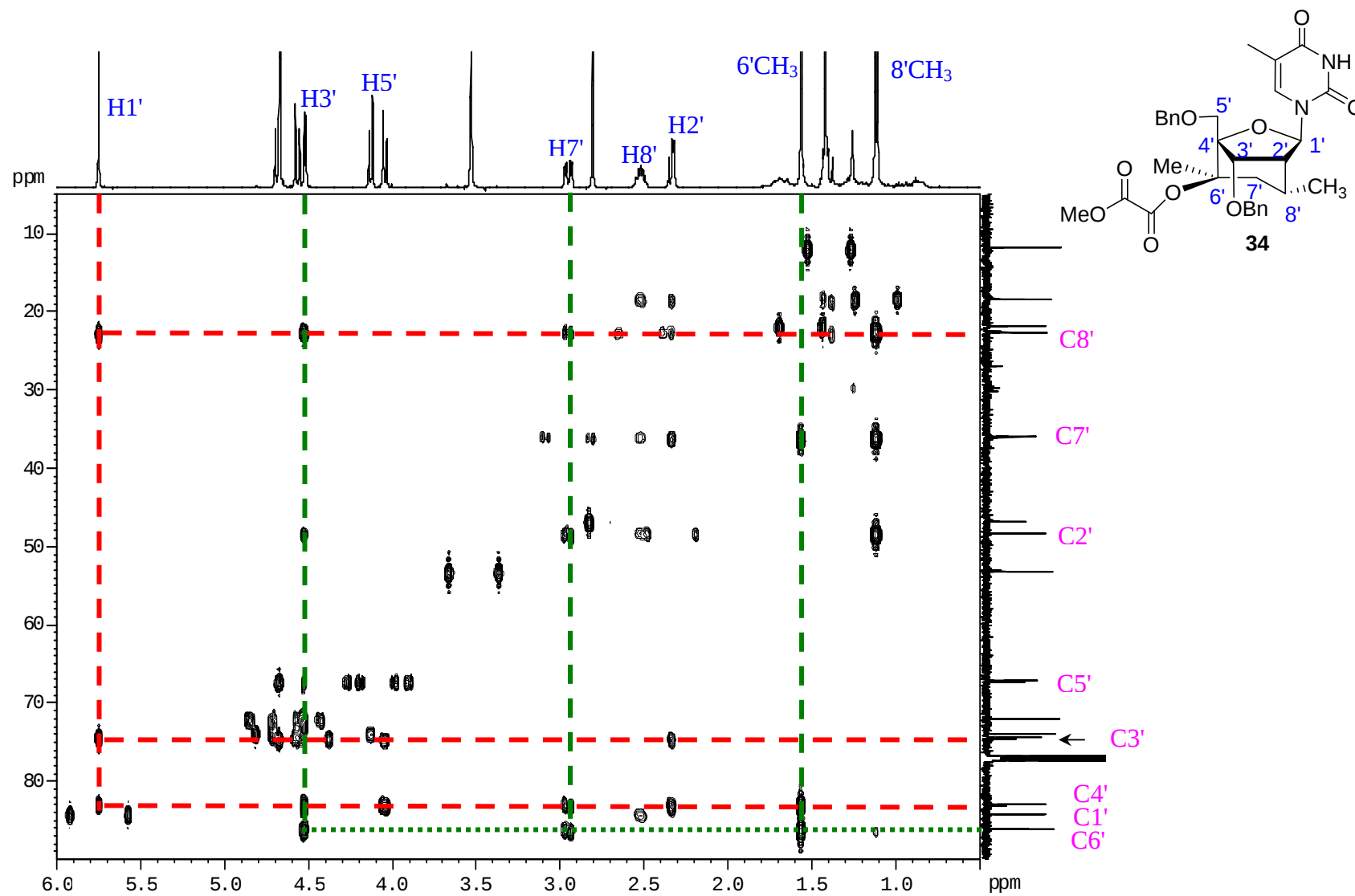


Figure SII.29. HMBC spectrum of compound 34.

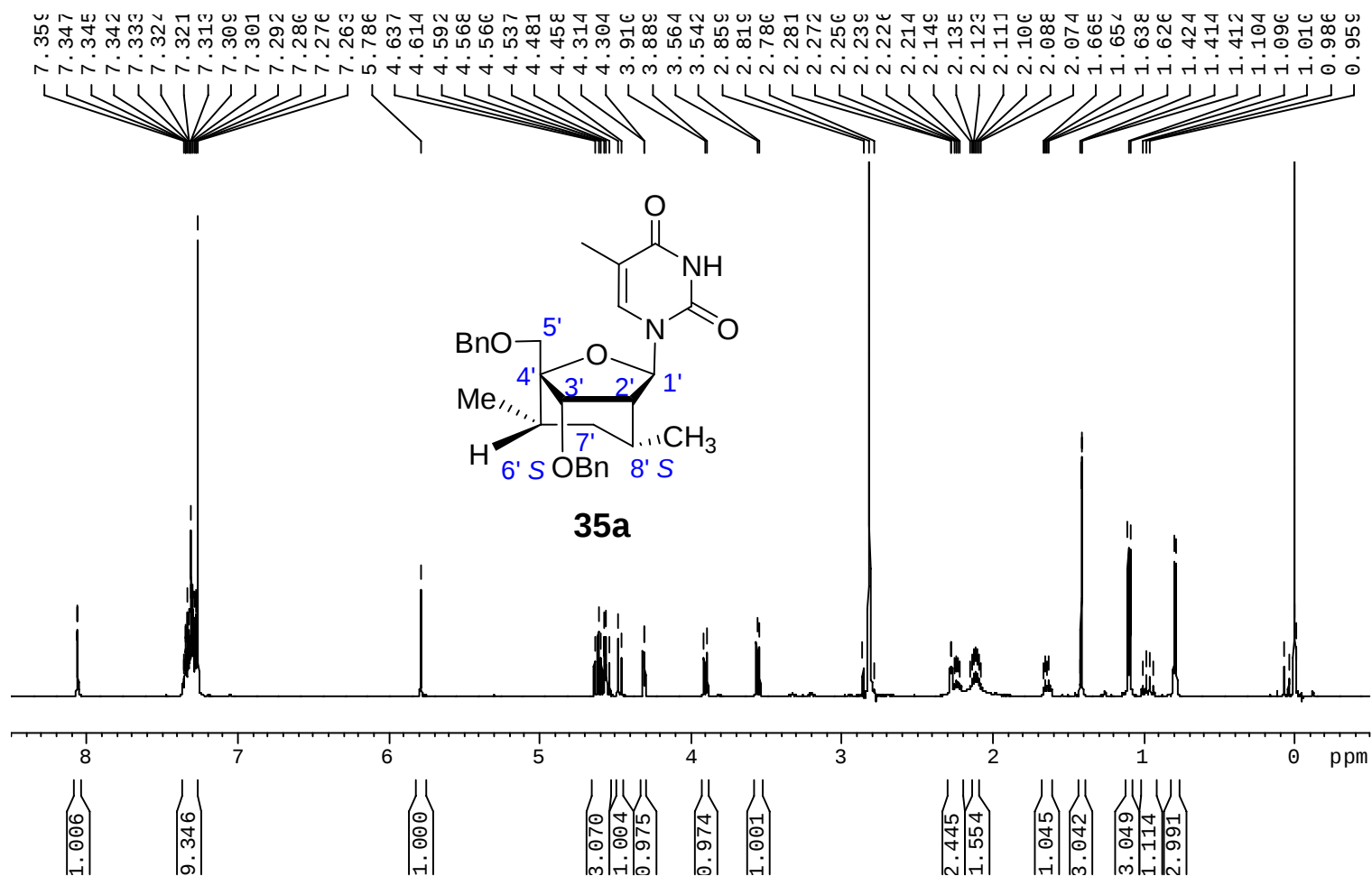


Figure SII.30. ^1H NMR spectrum of compound 35a.

Figure SII.31. ^{13}C NMR spectrum of compound 35a.

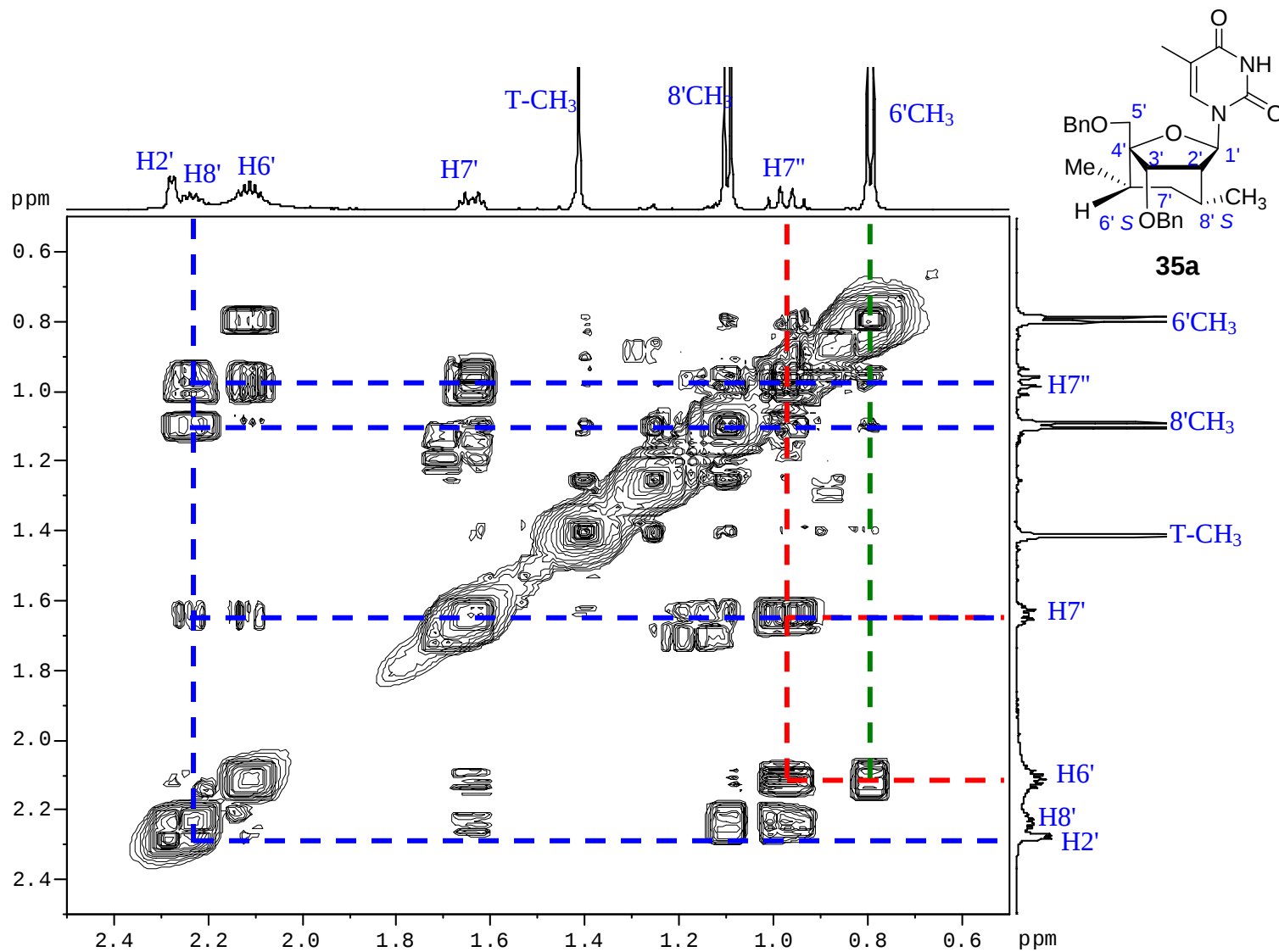


Figure SII.32. COSY spectrum of compound 35a.

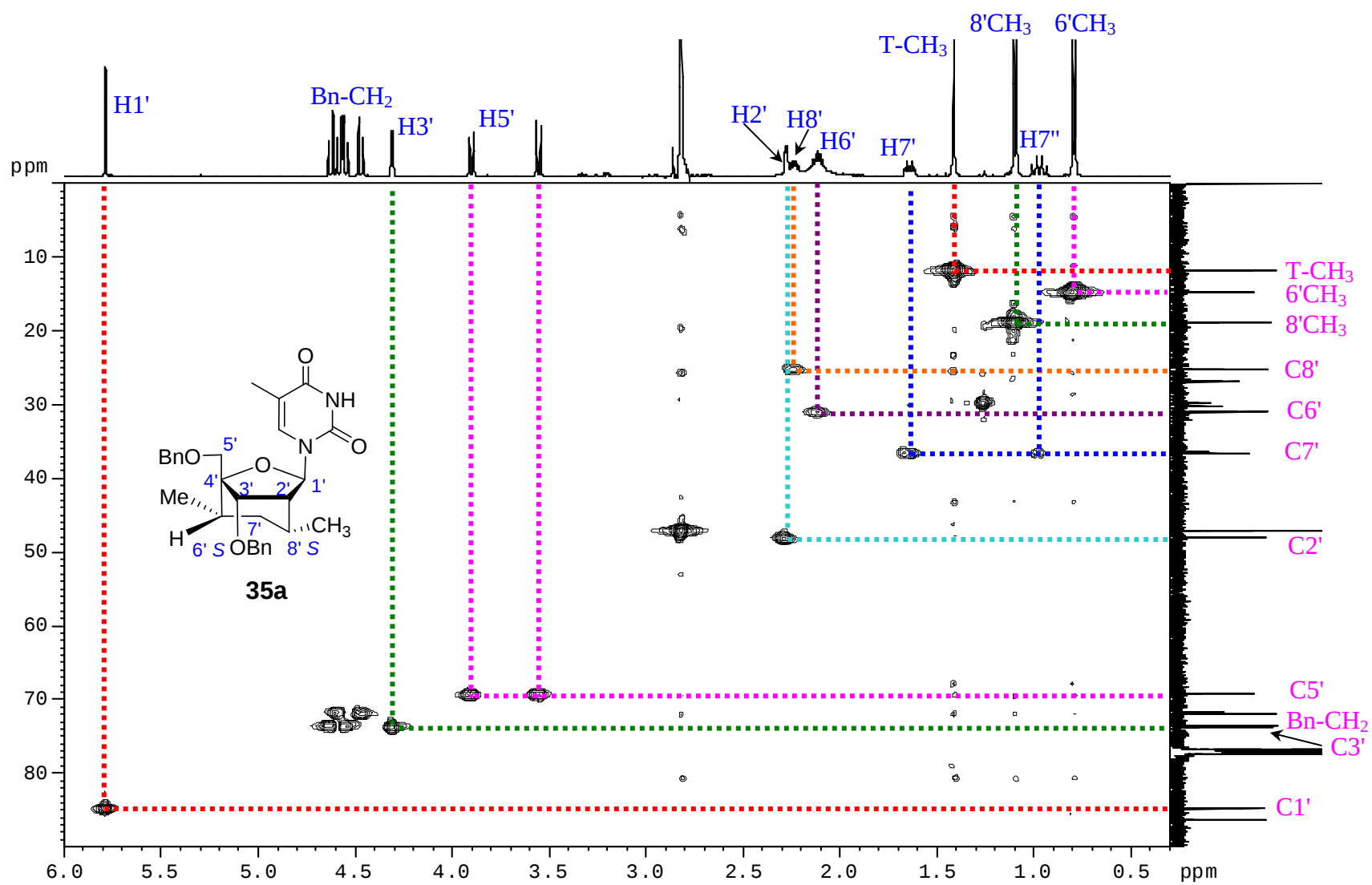


Figure SII.33. HMBC spectrum of compound 35a.

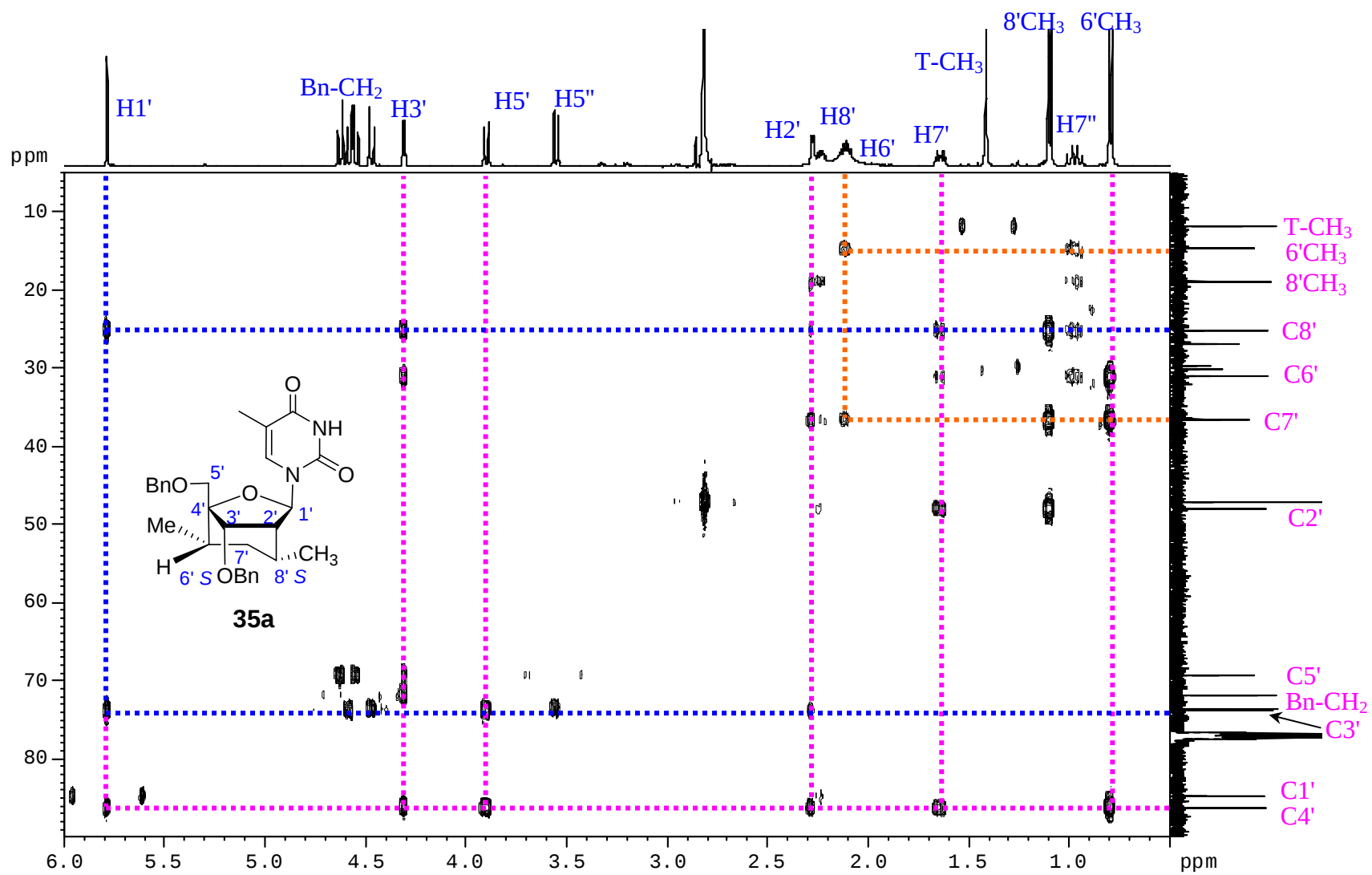


Figure SII.34. HMBC spectrum of compound 35a.

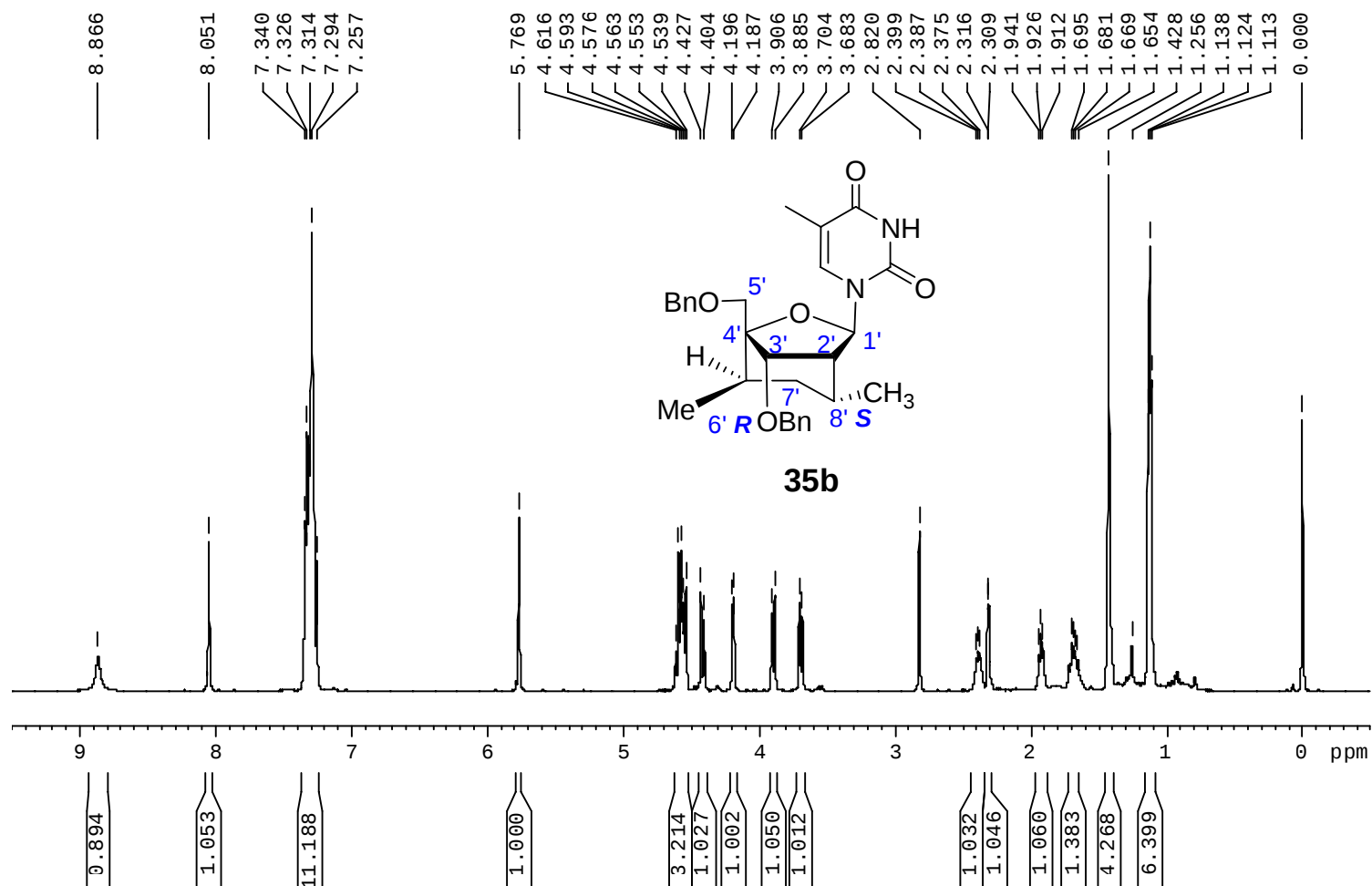


Figure SII.35. ^1H NMR spectrum of compound **35b**.

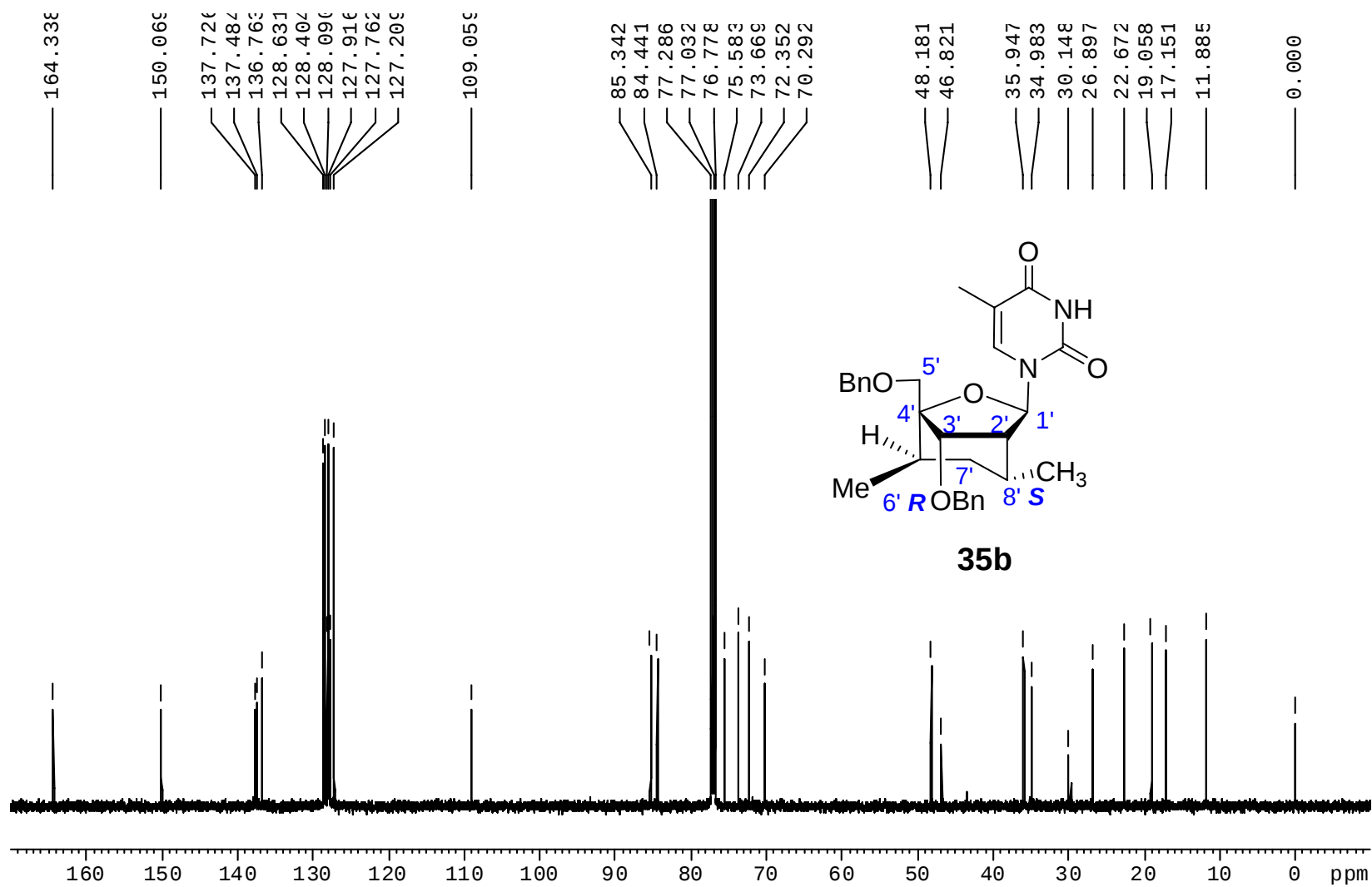
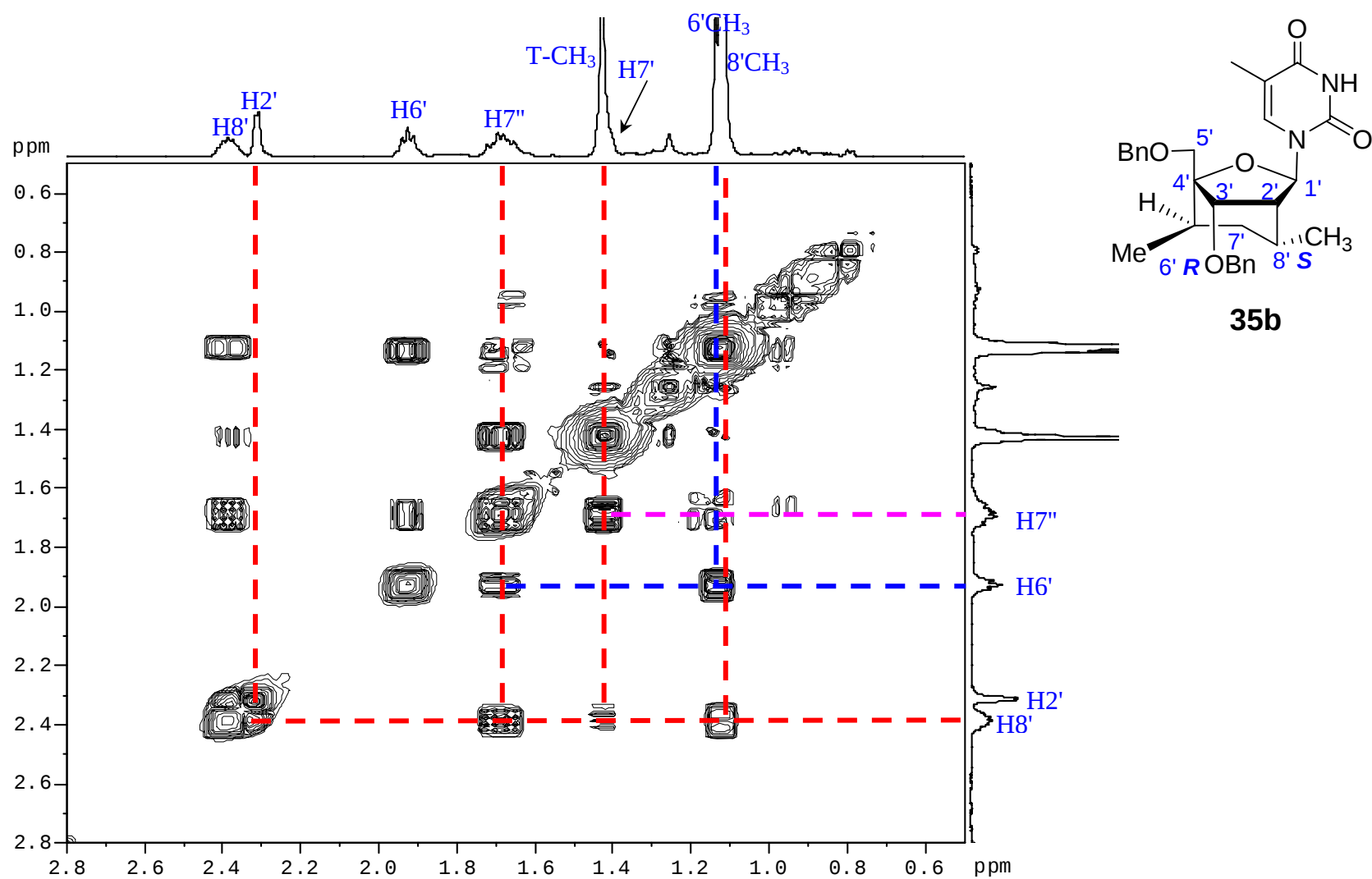
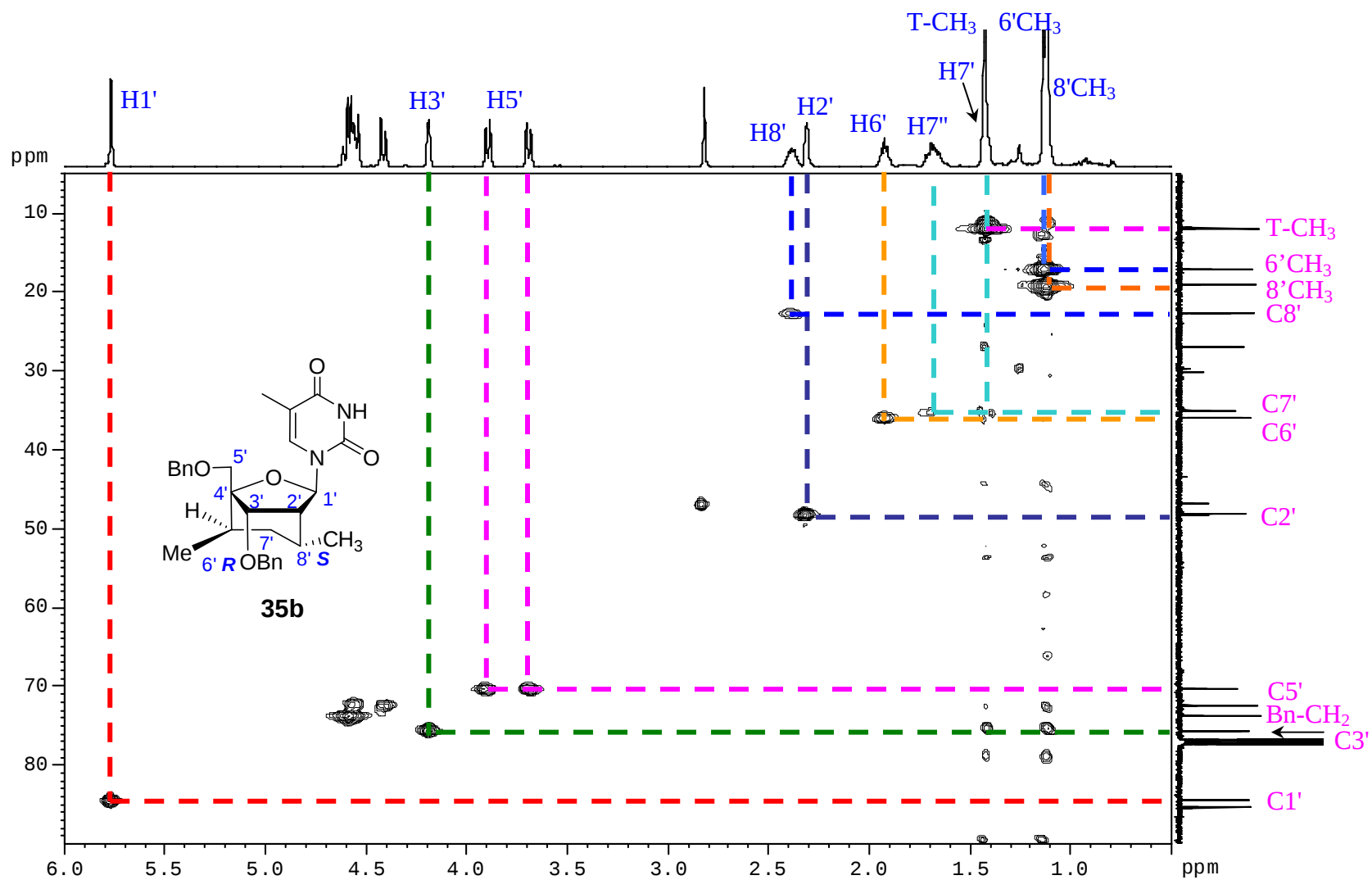
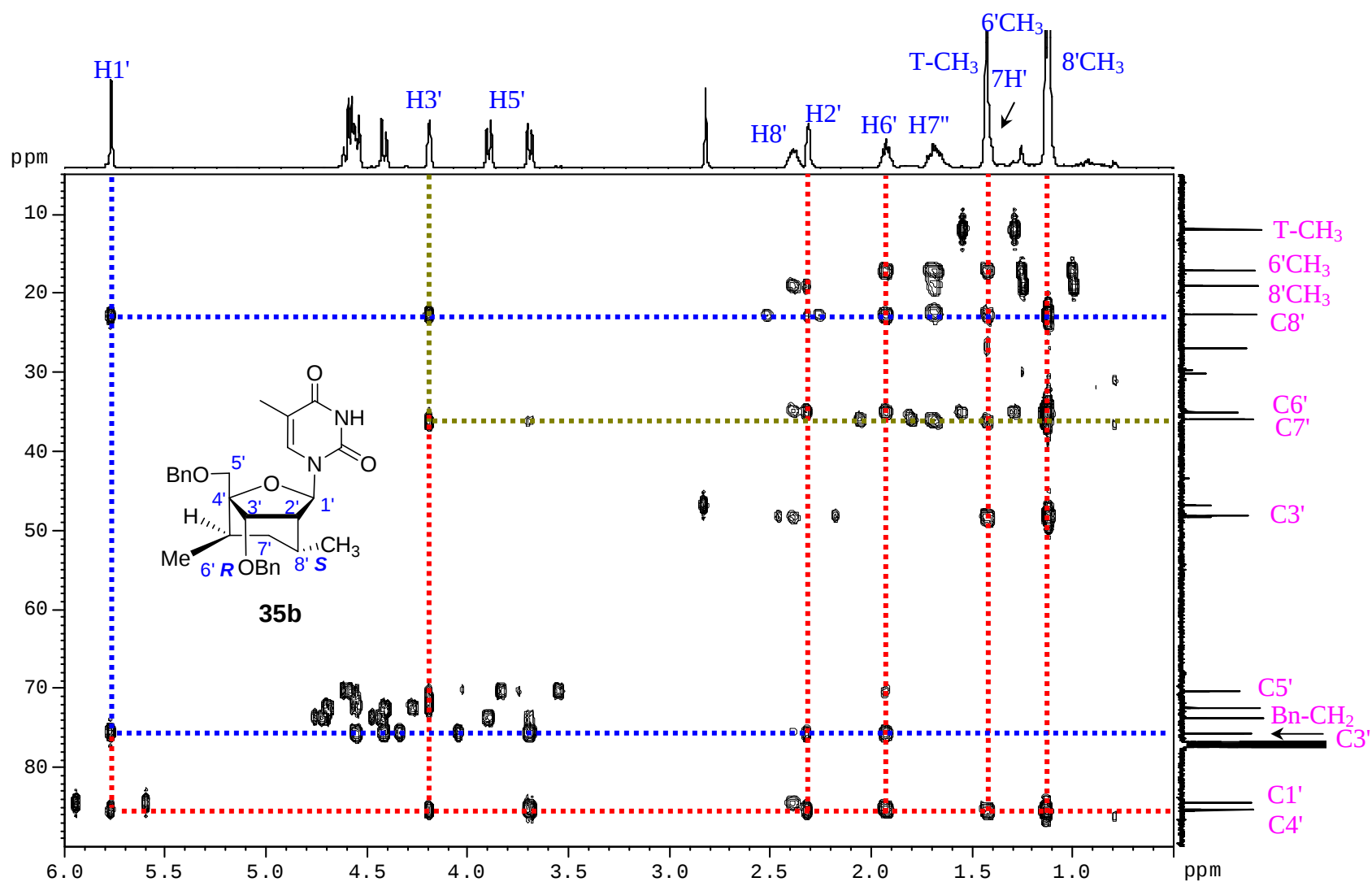


Figure SII.36. ¹³C NMR spectrum of compound 35b.

Figure SII.37. COSY spectrum of compound **35b**.

Figure SII.38. HMQC spectrum of compound **35b**.

Figure SII.39. HMBC spectrum of compound **35b**.

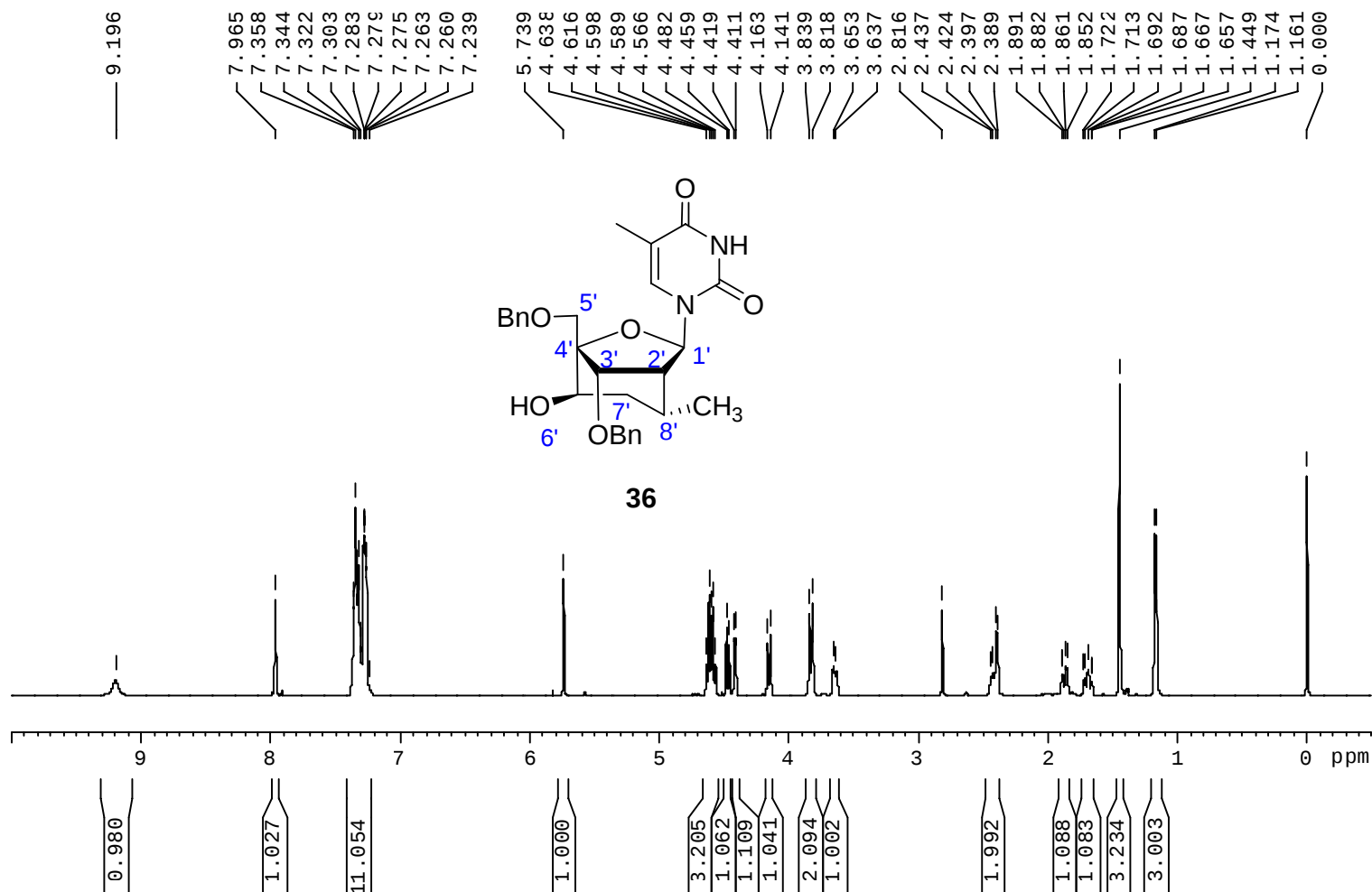


Figure SII.40. ¹H NMR spectrum of compound 36.

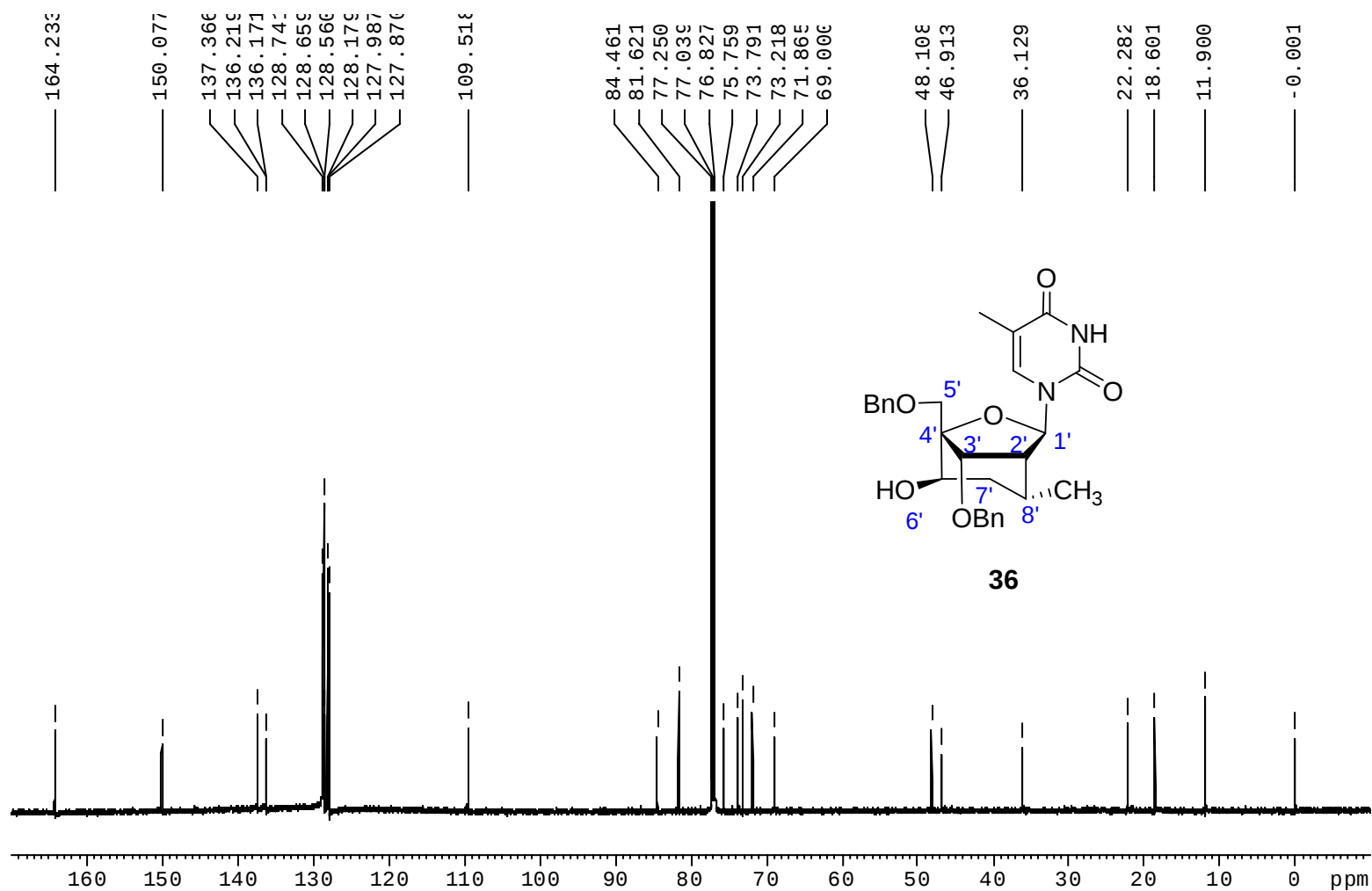


Figure SII.41. ^{13}C NMR spectrum of compound 36.

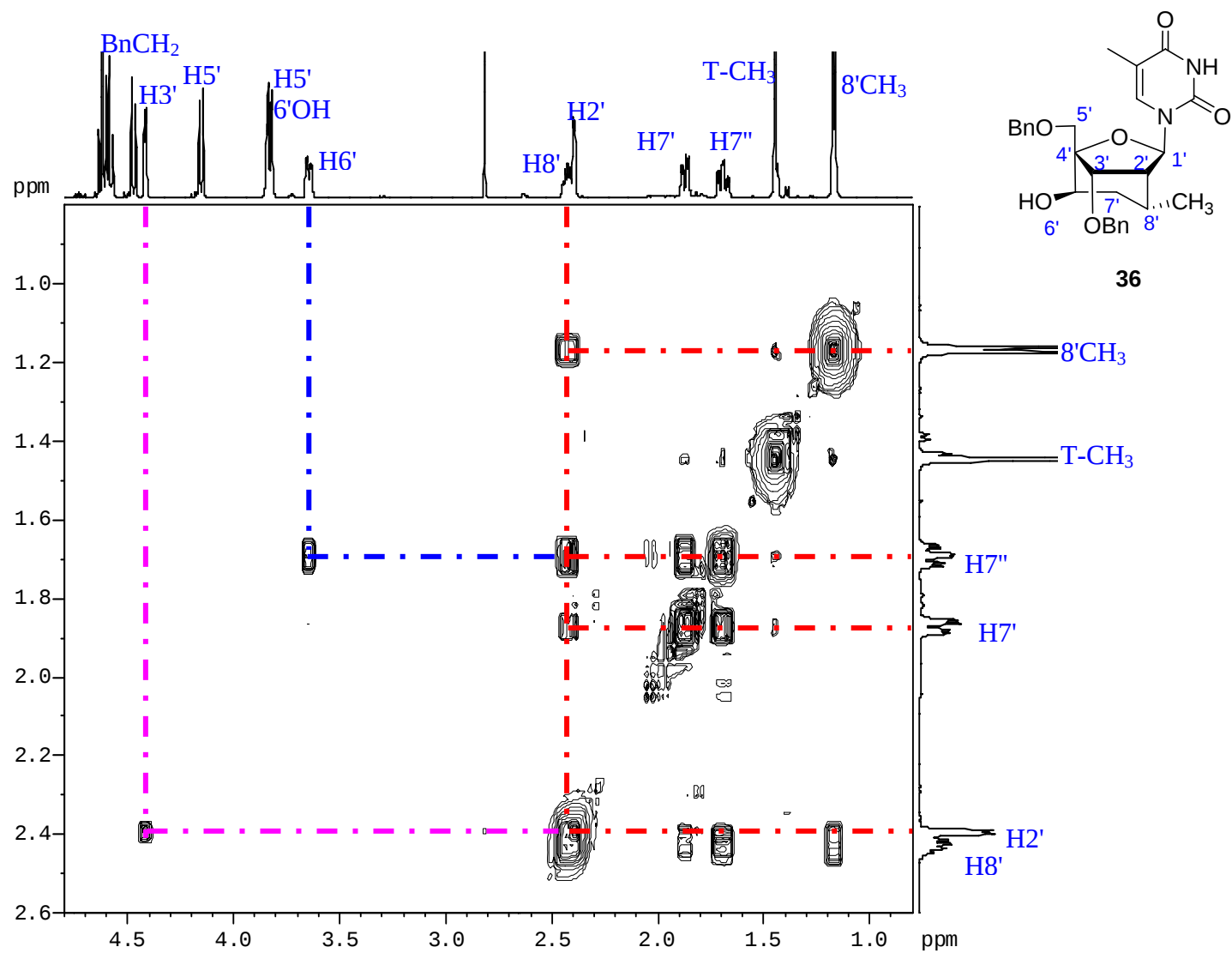


Figure SII.42. COSY spectrum of compound 36.

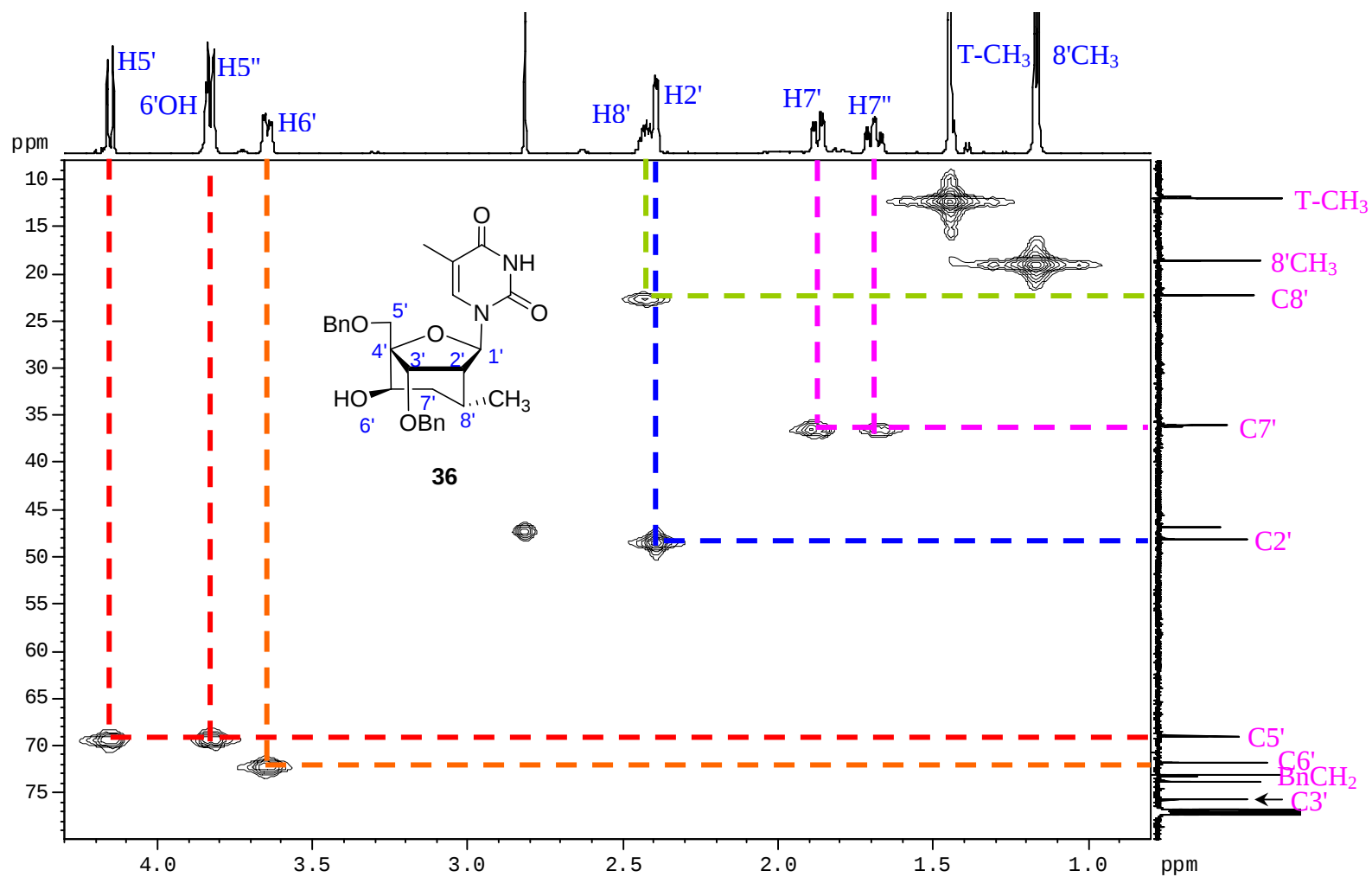


Figure SII.43. HMQC spectrum of compound 36.

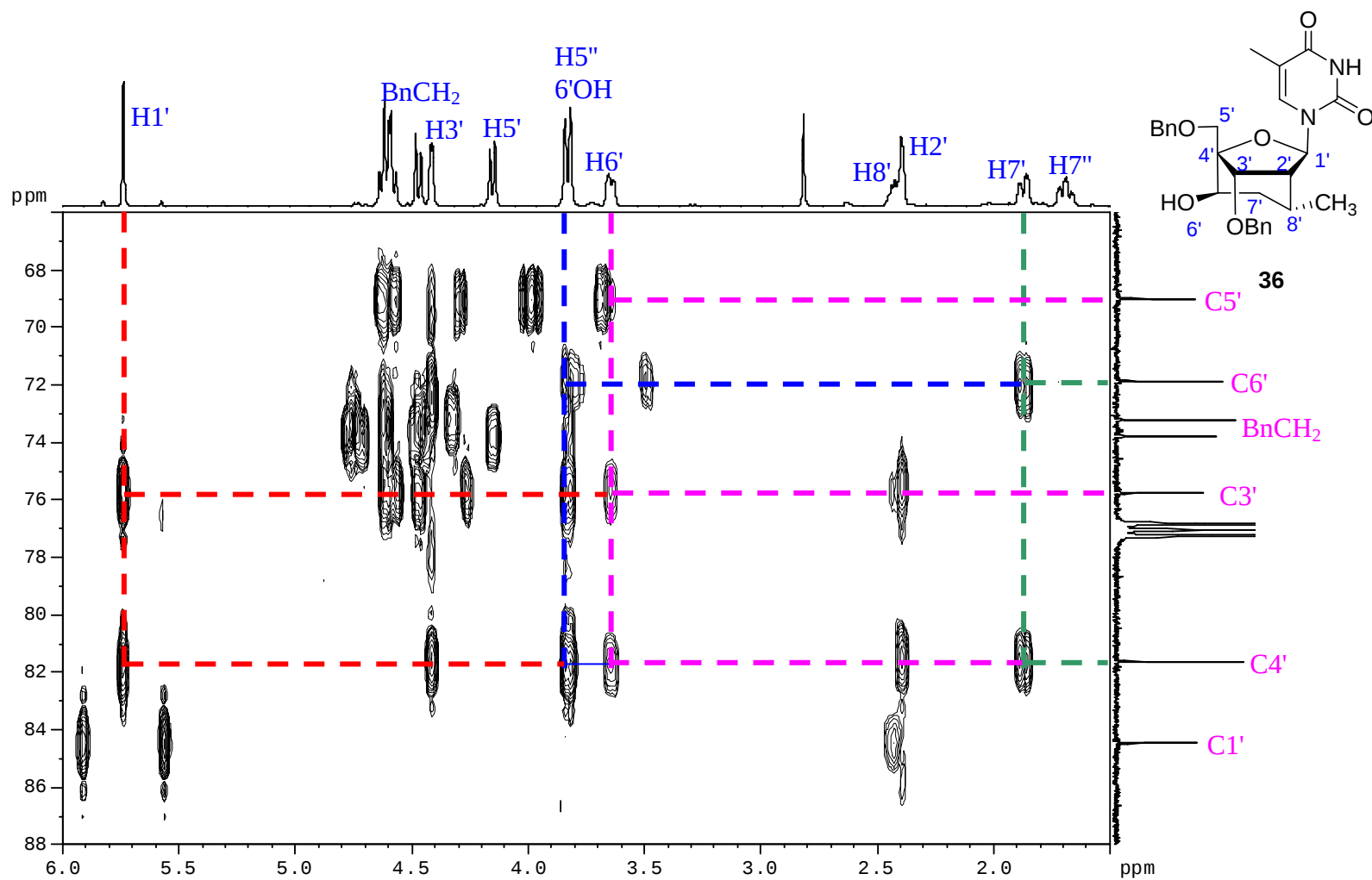


Figure SII.44. HMBC spectrum of compound 36.

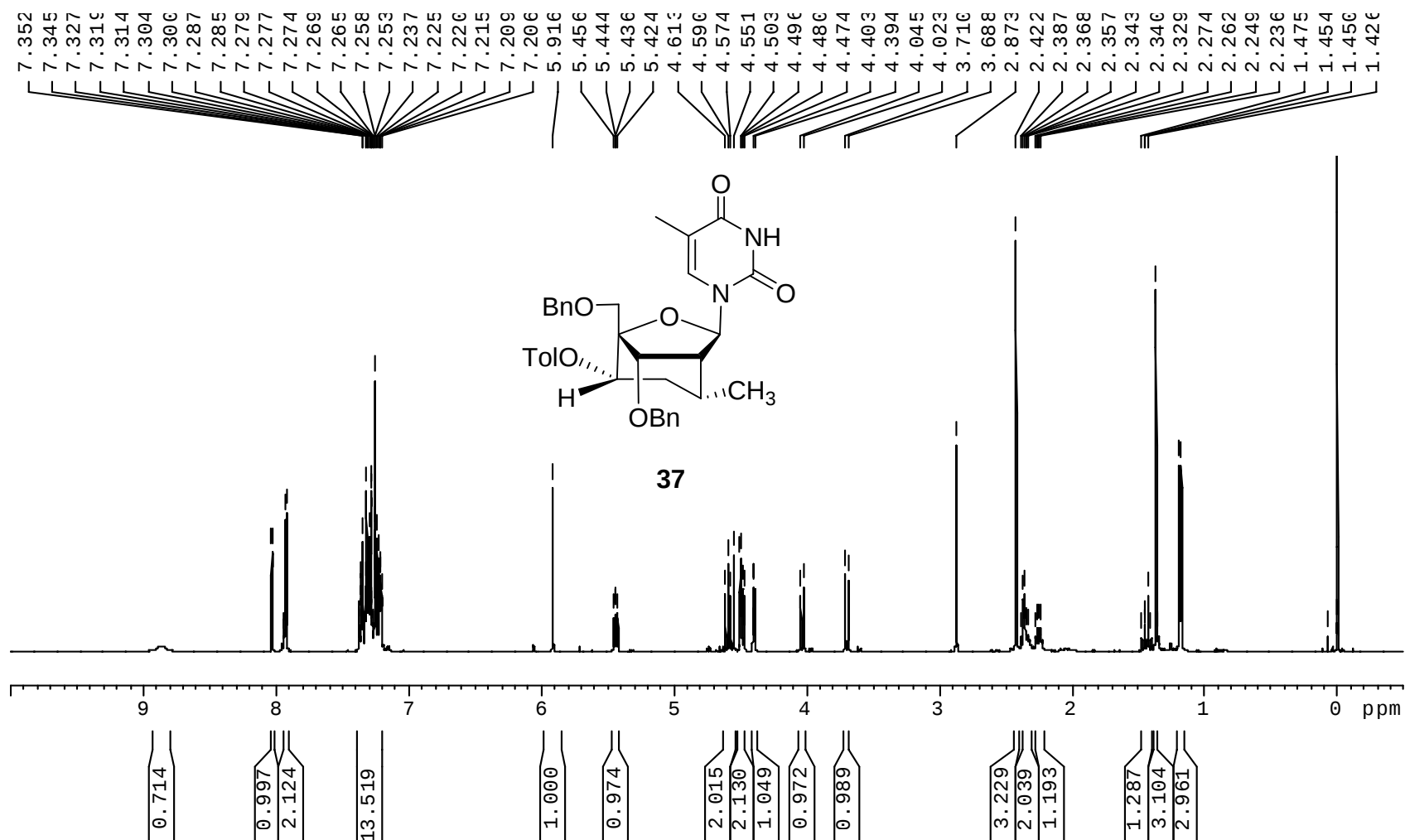


Figure SII.45. ¹H NMR spectrum of compound 37.

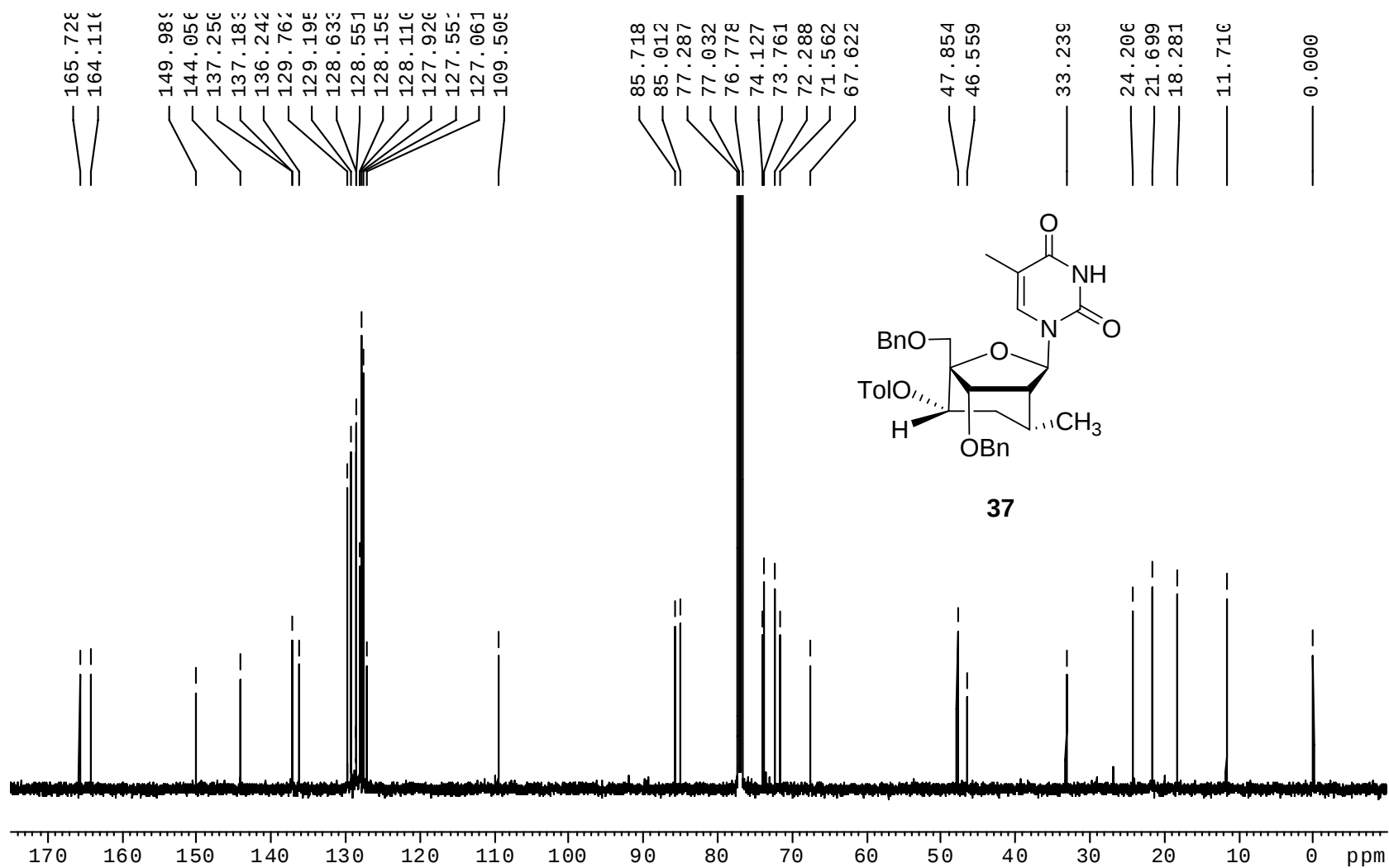


Figure SII.46. ¹³C NMR spectrum of compound 37.

Figure SII.47. ^1H NMR spectrum of compound 38.

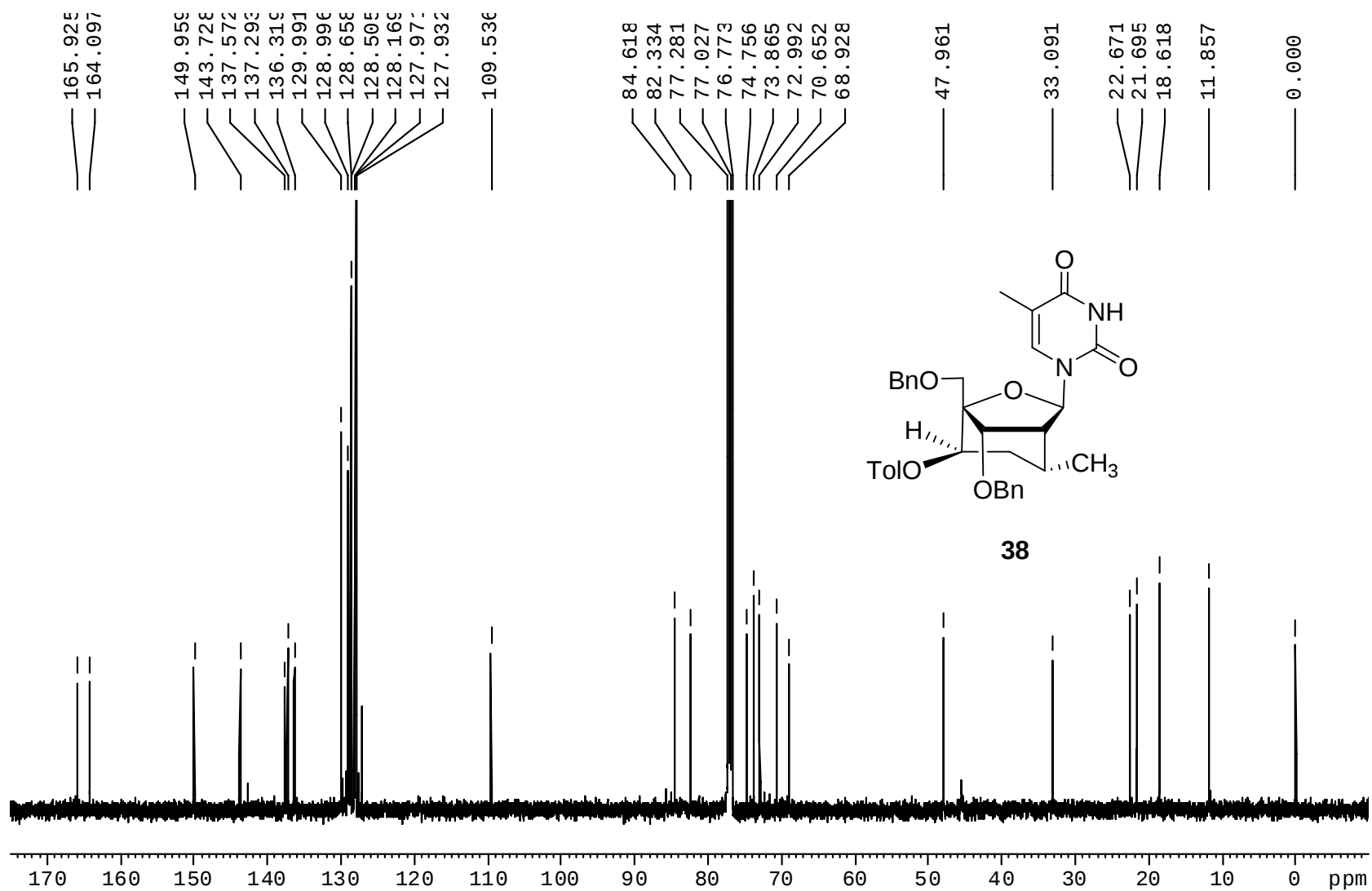


Figure SII.48. ¹³C NMR spectrum of compound 38.

Figure SII.49. ^1H NMR spectrum of compound 39.

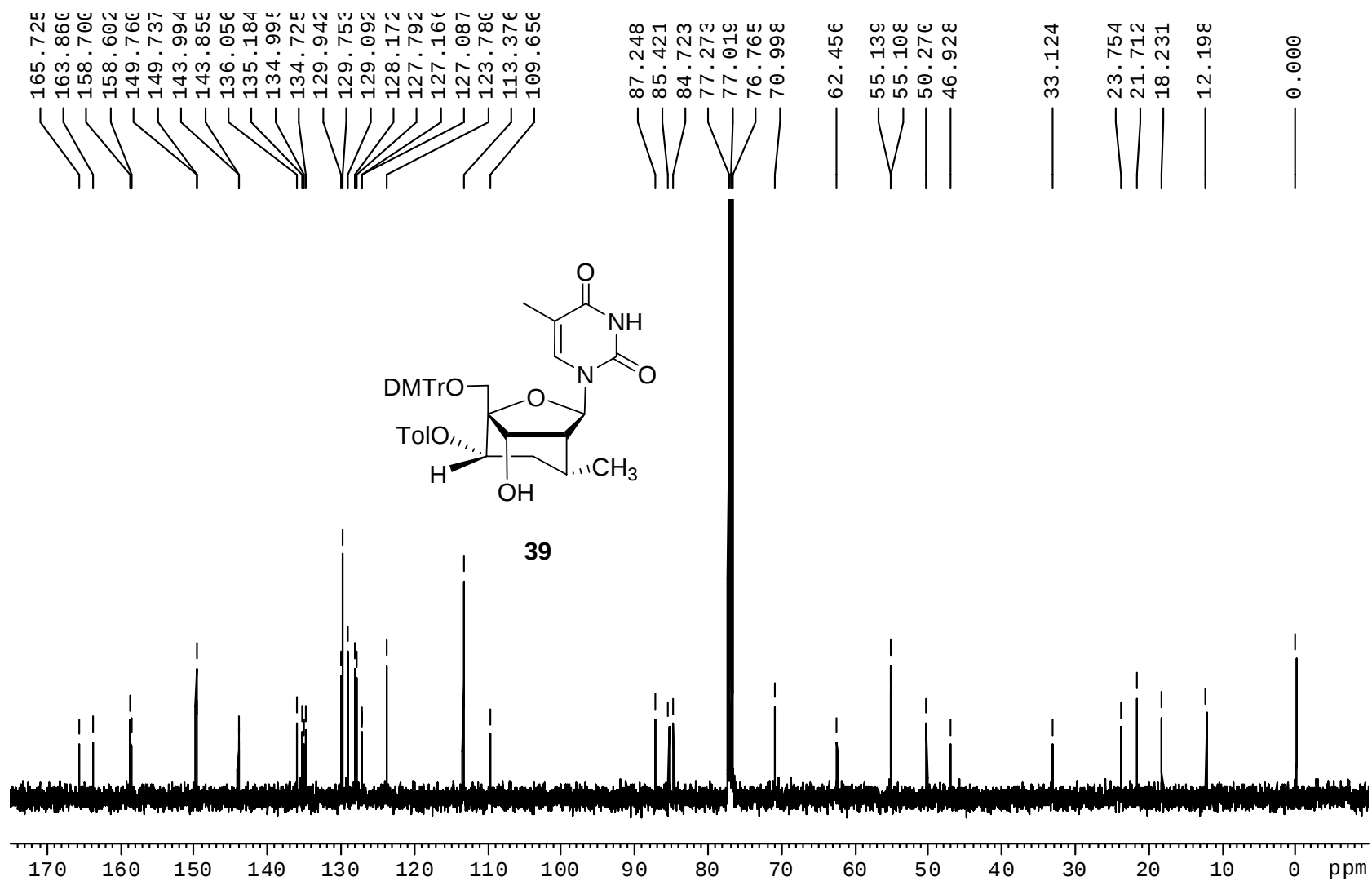


Figure SII.50. ¹³C NMR spectrum of compound 39.

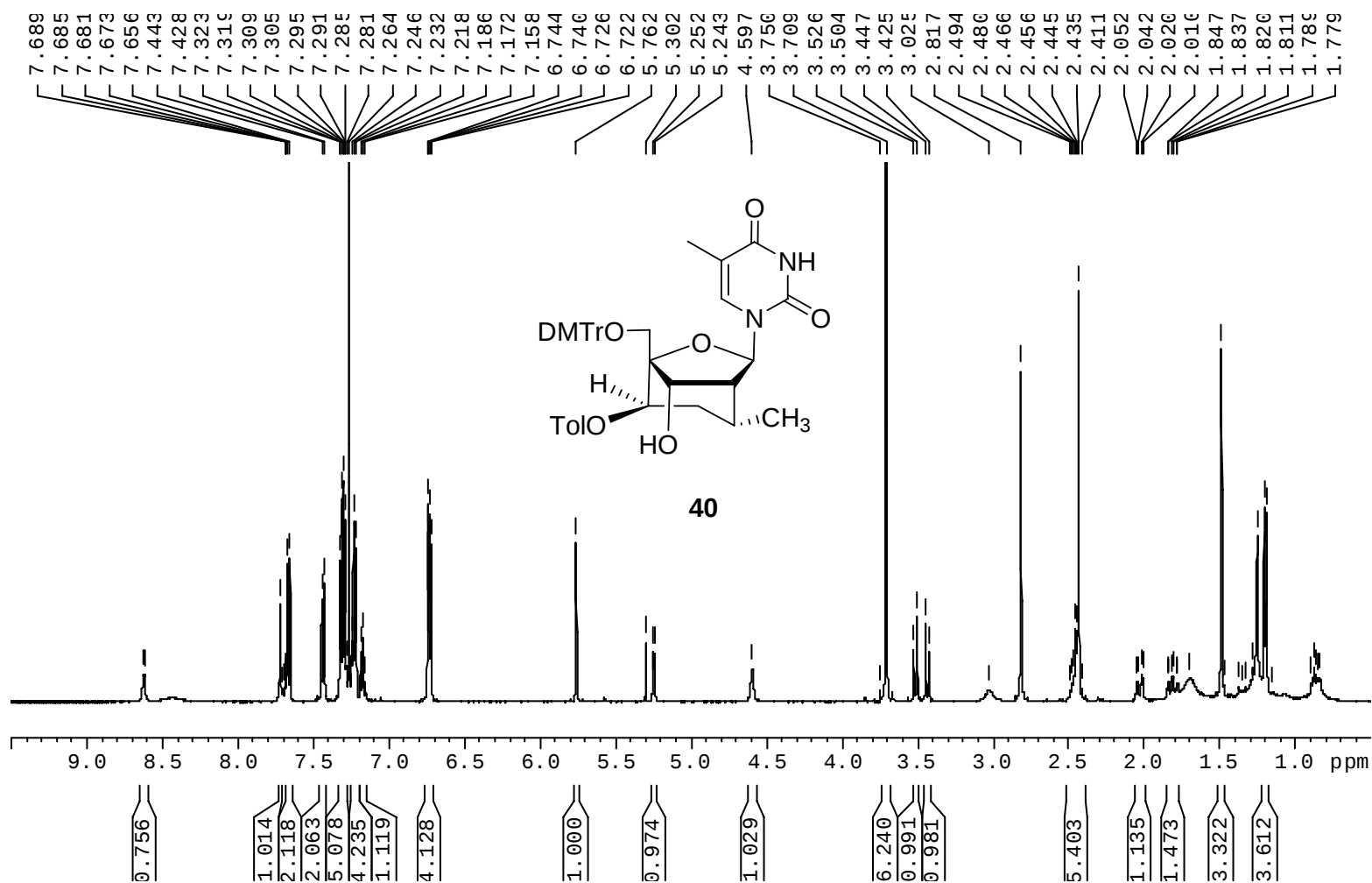


Figure SII.51. ¹H NMR spectrum of compound 40.

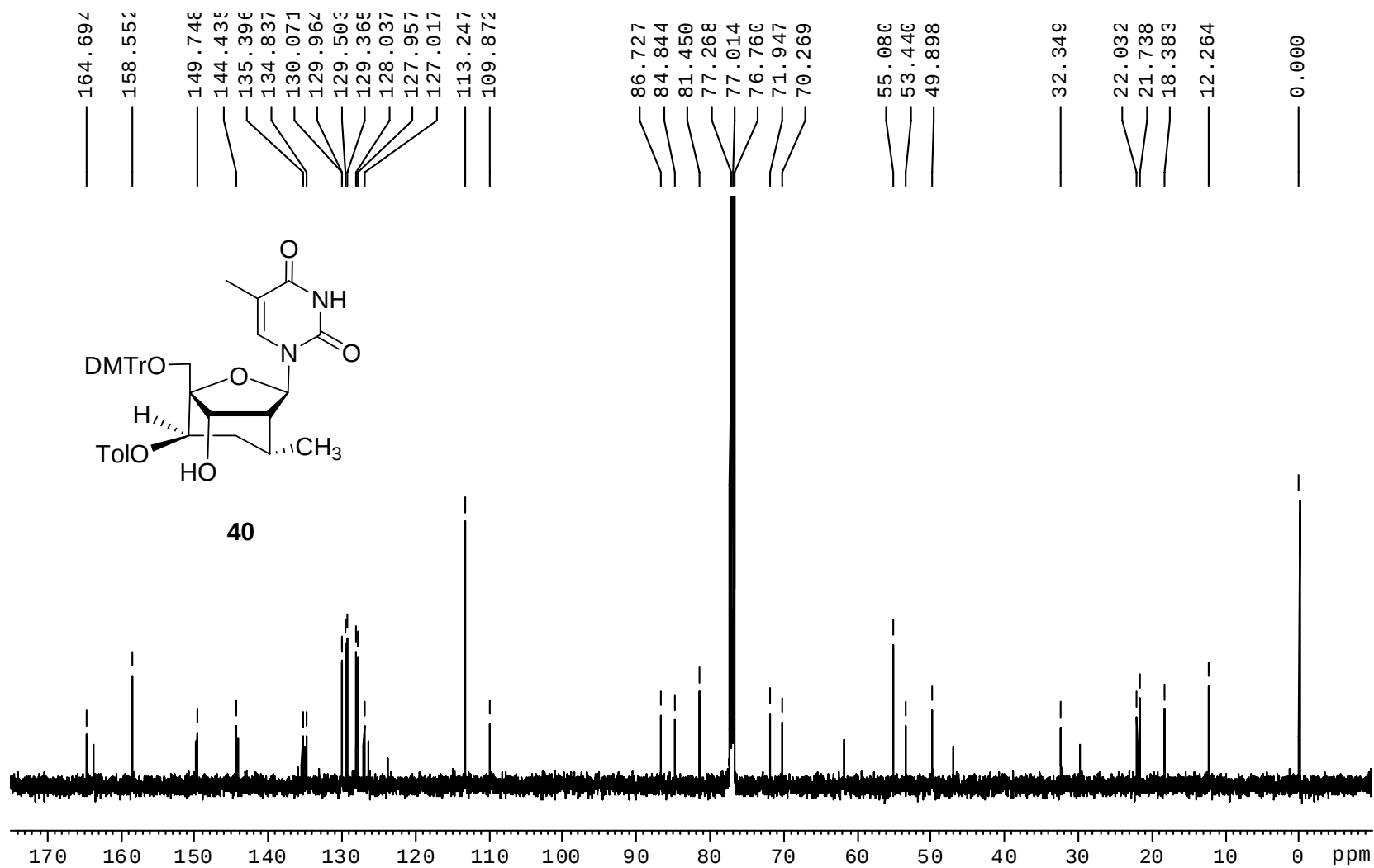


Figure SII.52. ¹³C NMR spectrum of compound 40.

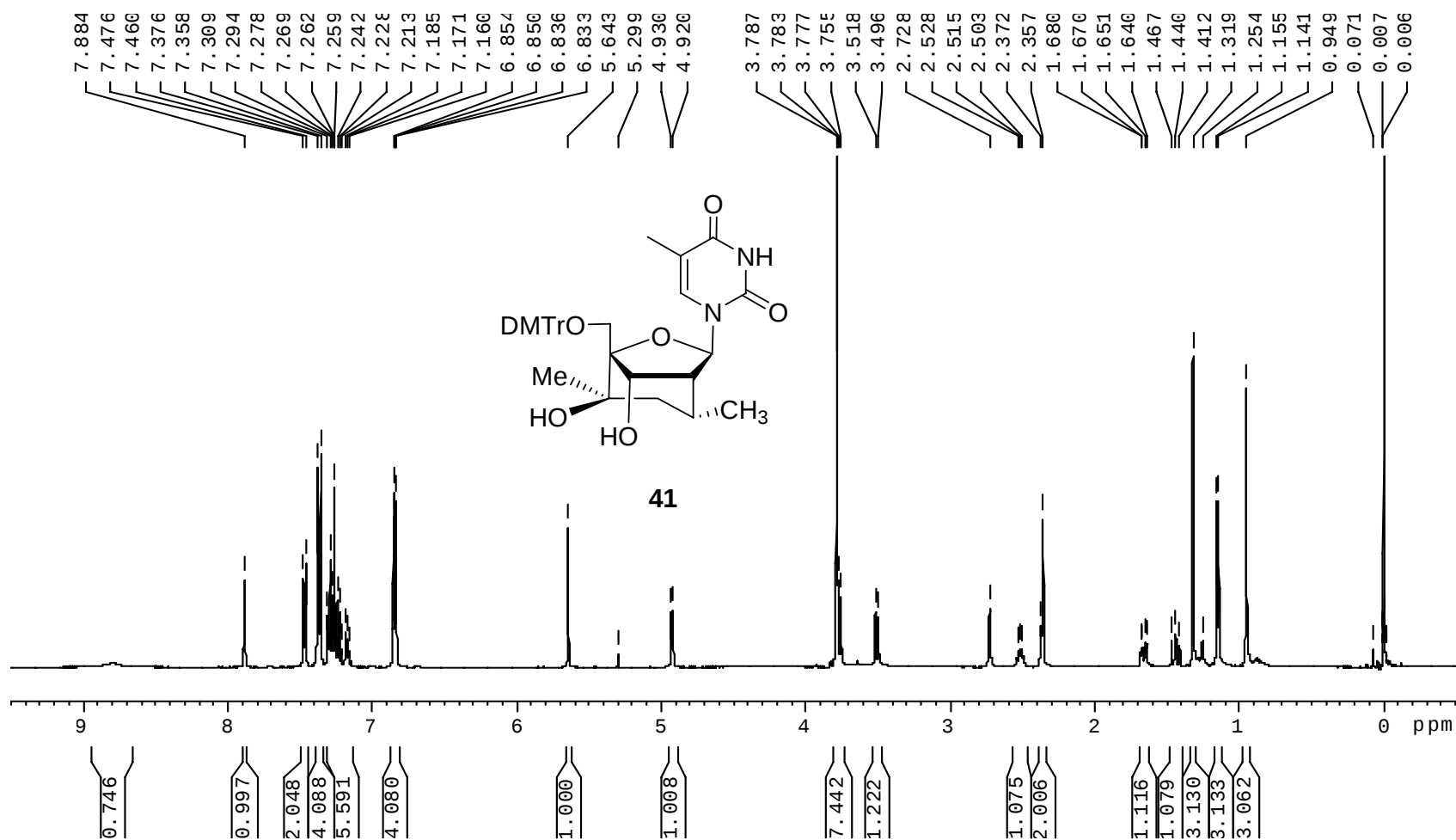


Figure SII.53. ^1H NMR spectrum of compound 41.

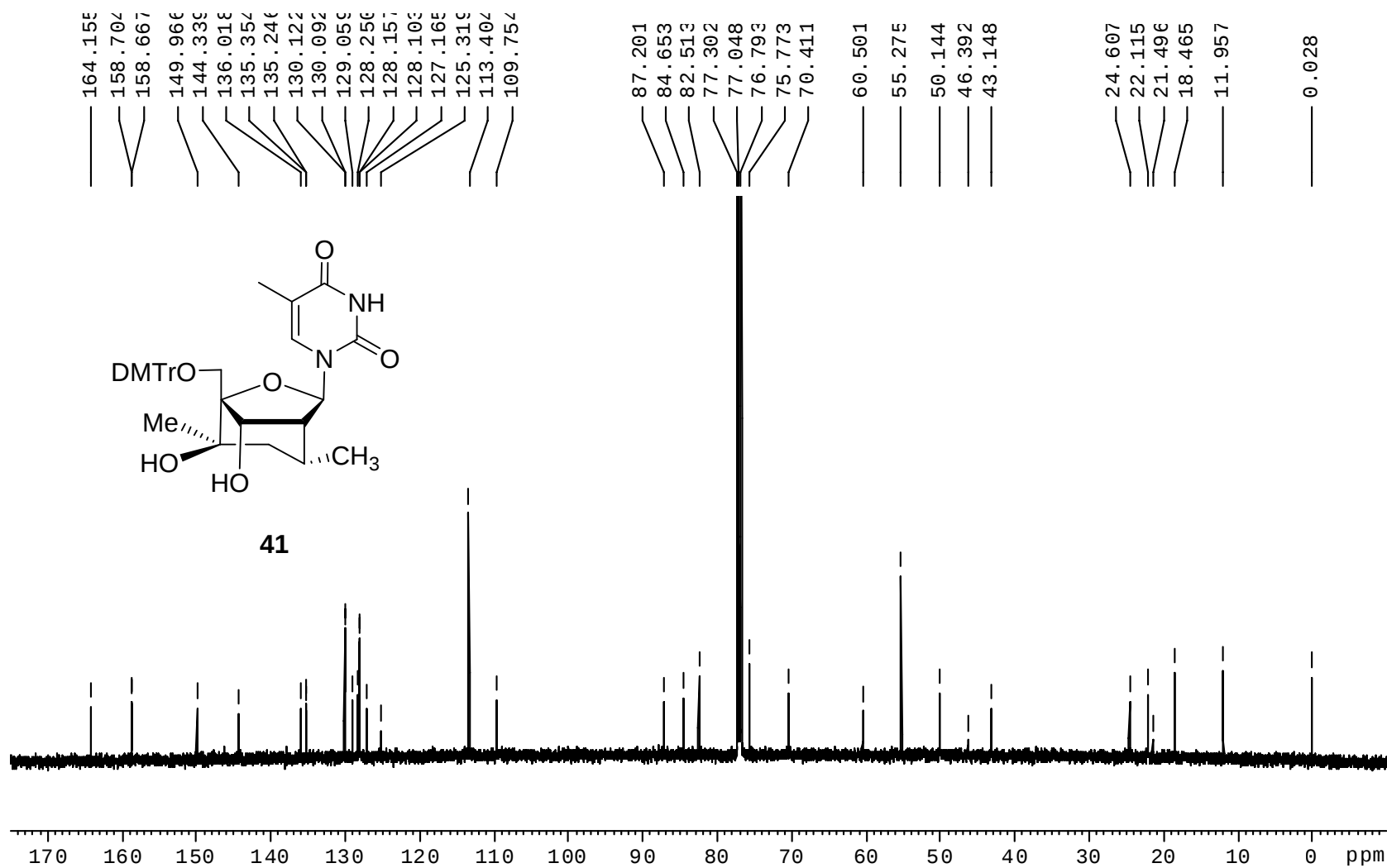


Figure SII.54. ^{13}C NMR spectrum of compound 41.

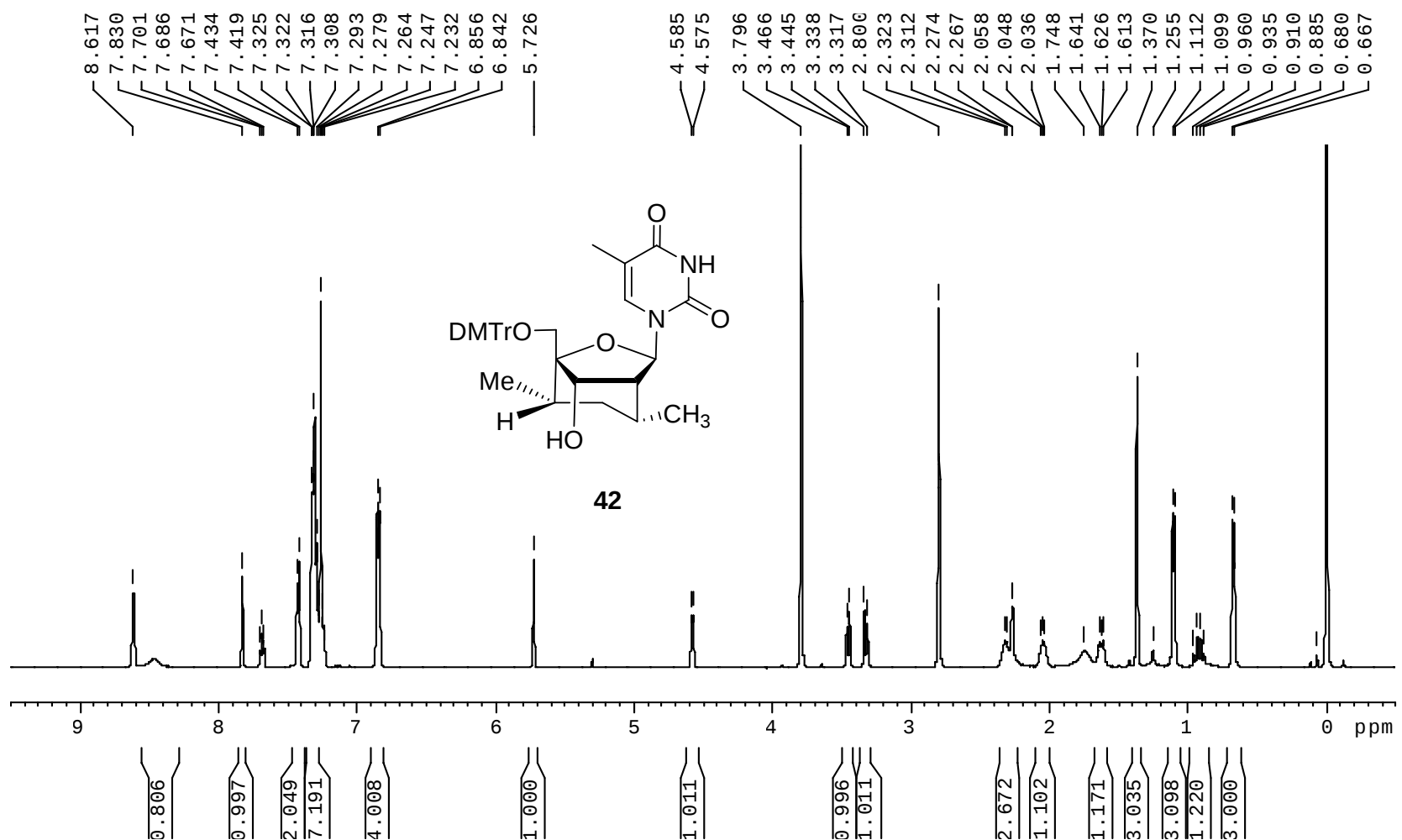


Figure SII.55. ¹H NMR spectrum of compound 42.

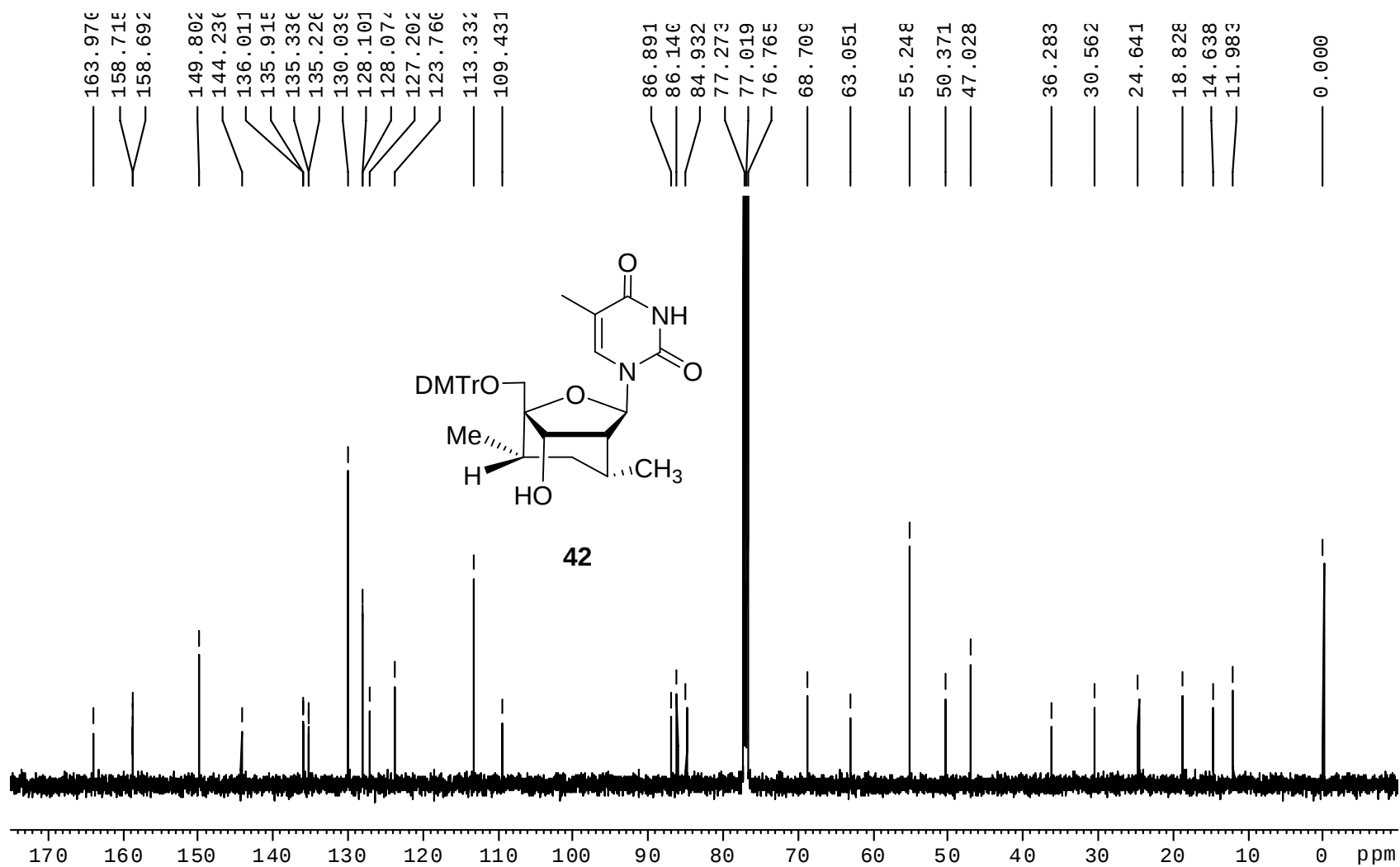


Figure SII.56. ¹³C NMR spectrum of compound 42.

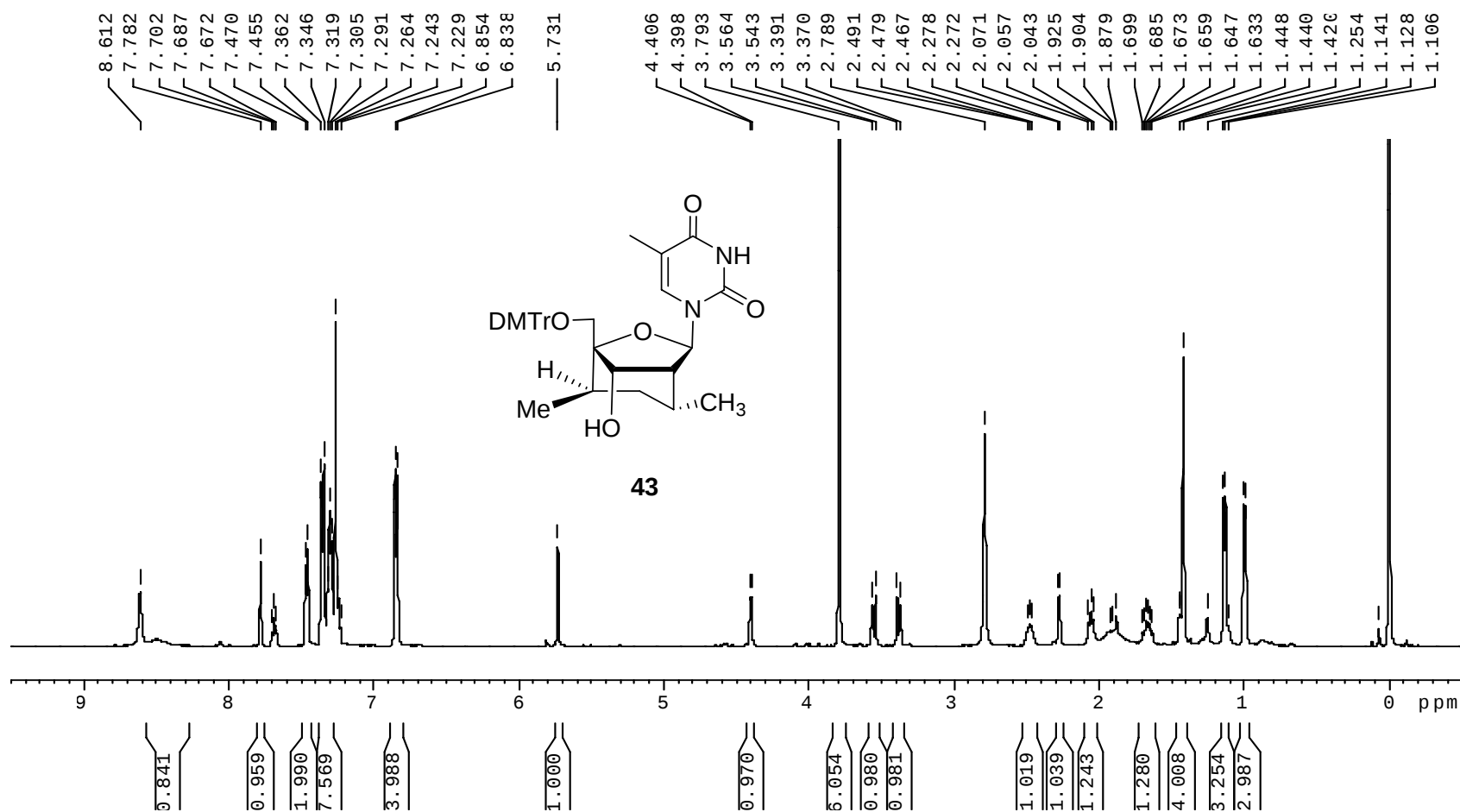


Figure SII.57. ^1H NMR spectrum of compound 43.

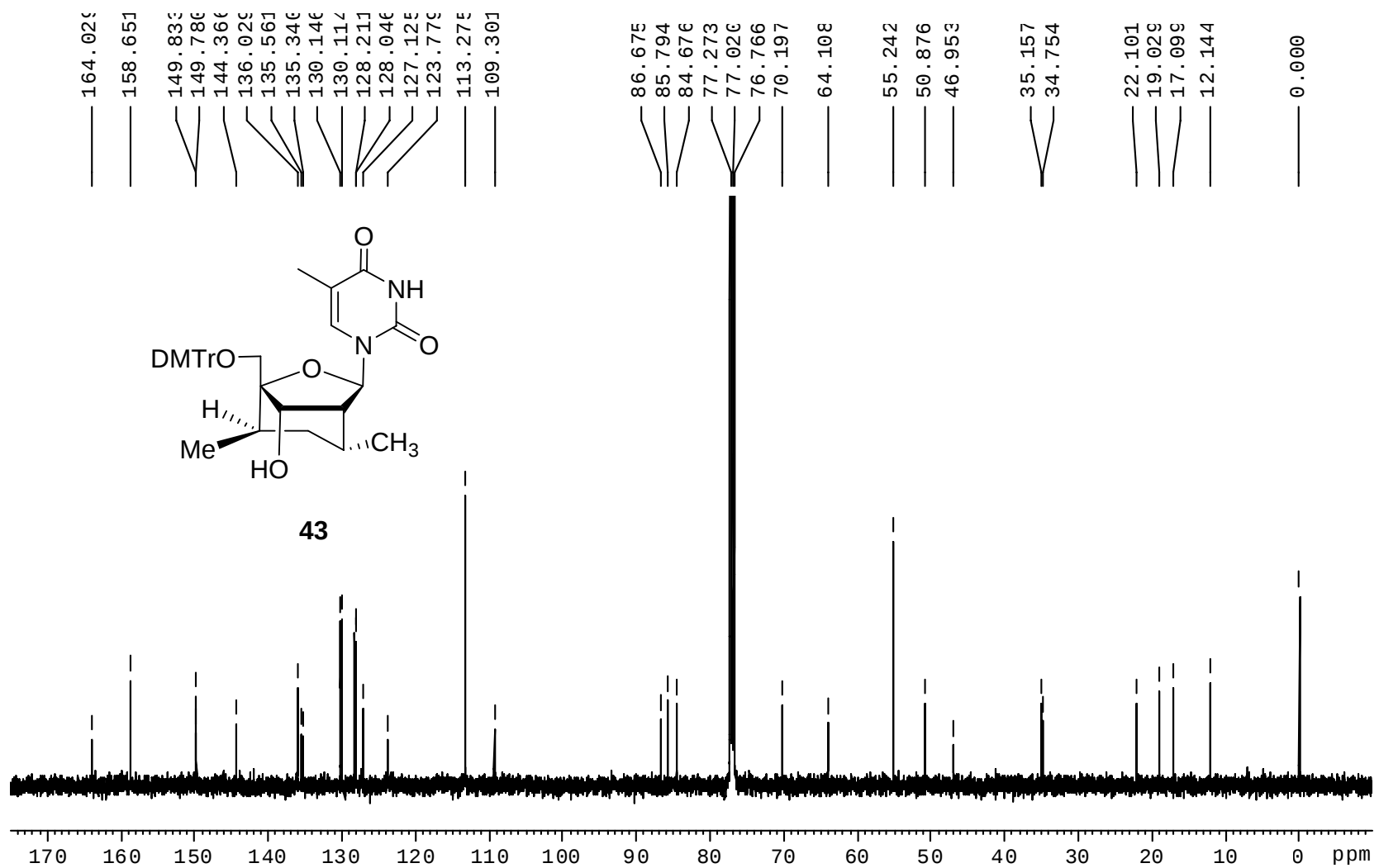


Figure SII.58. ¹³C NMR spectrum of compound 43.

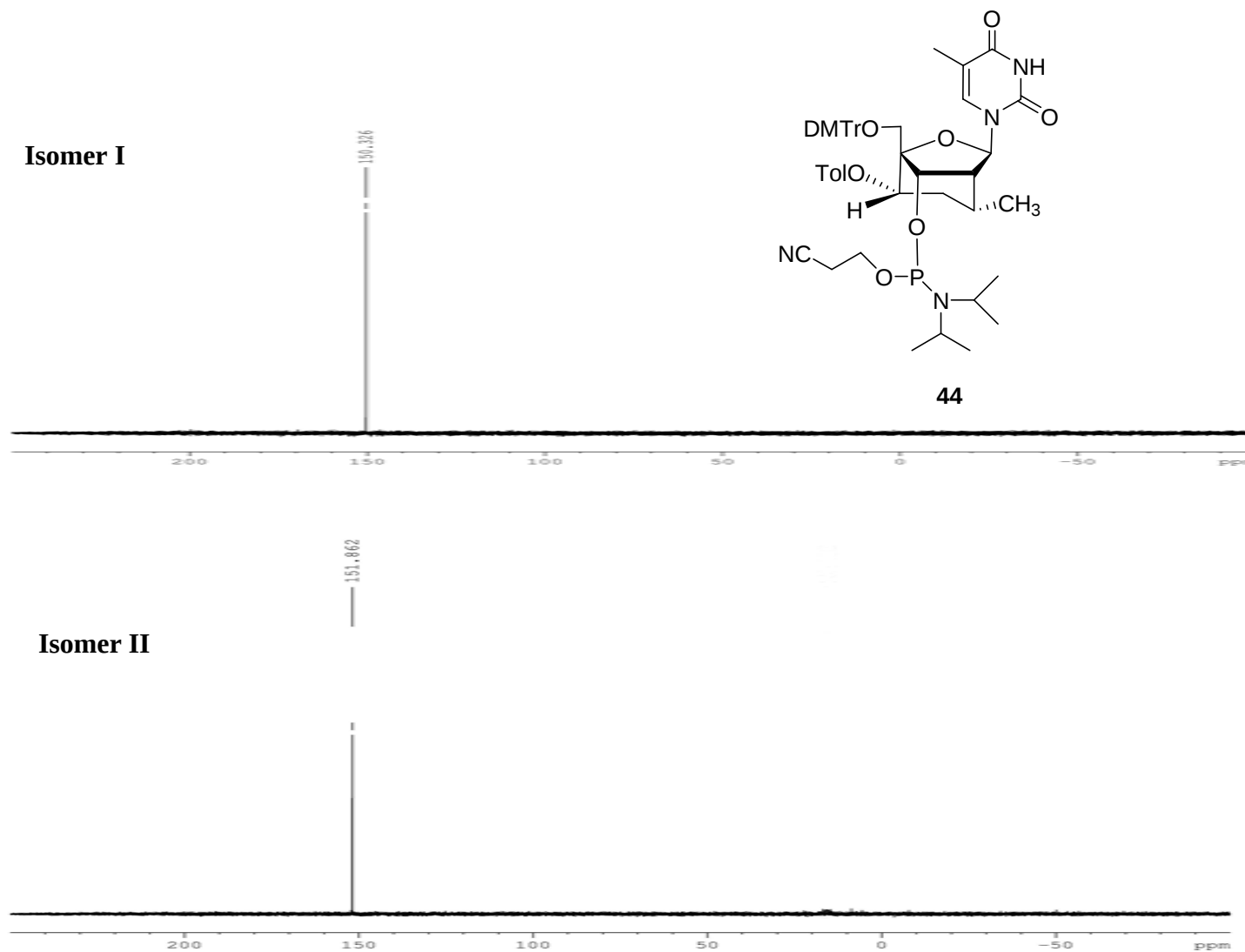
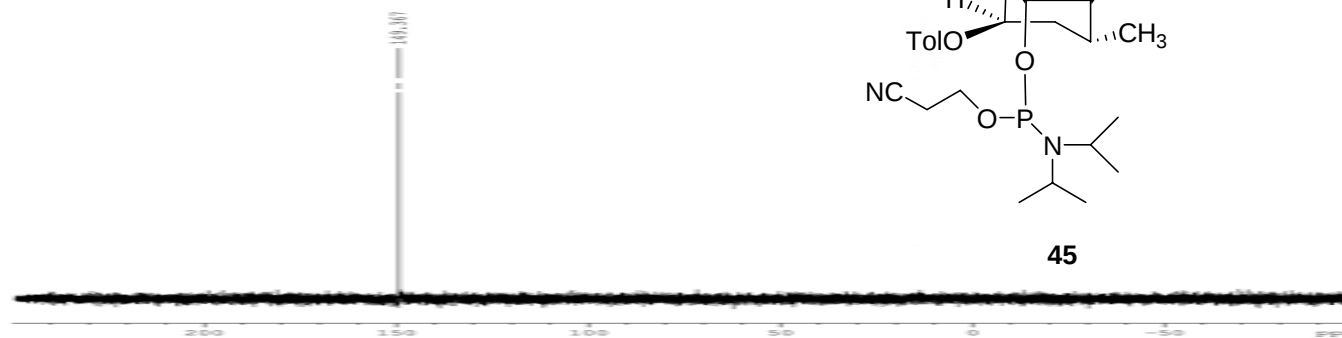
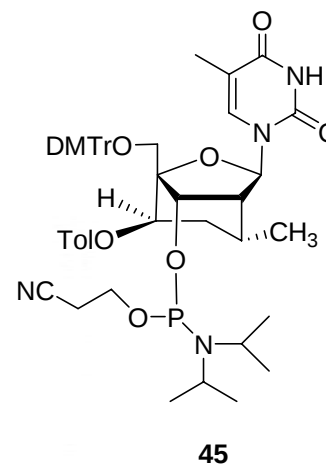


Figure SII.59. ^{31}P NMR spectrum of compound 44.

Isomer I



Isomer II

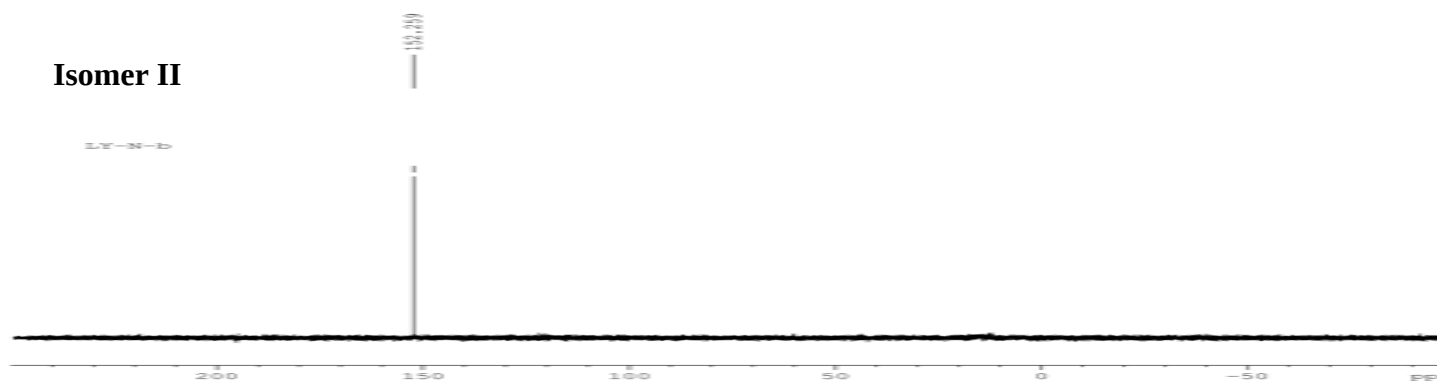


Figure SII.60. ^{31}P NMR spectrum of compound 45.

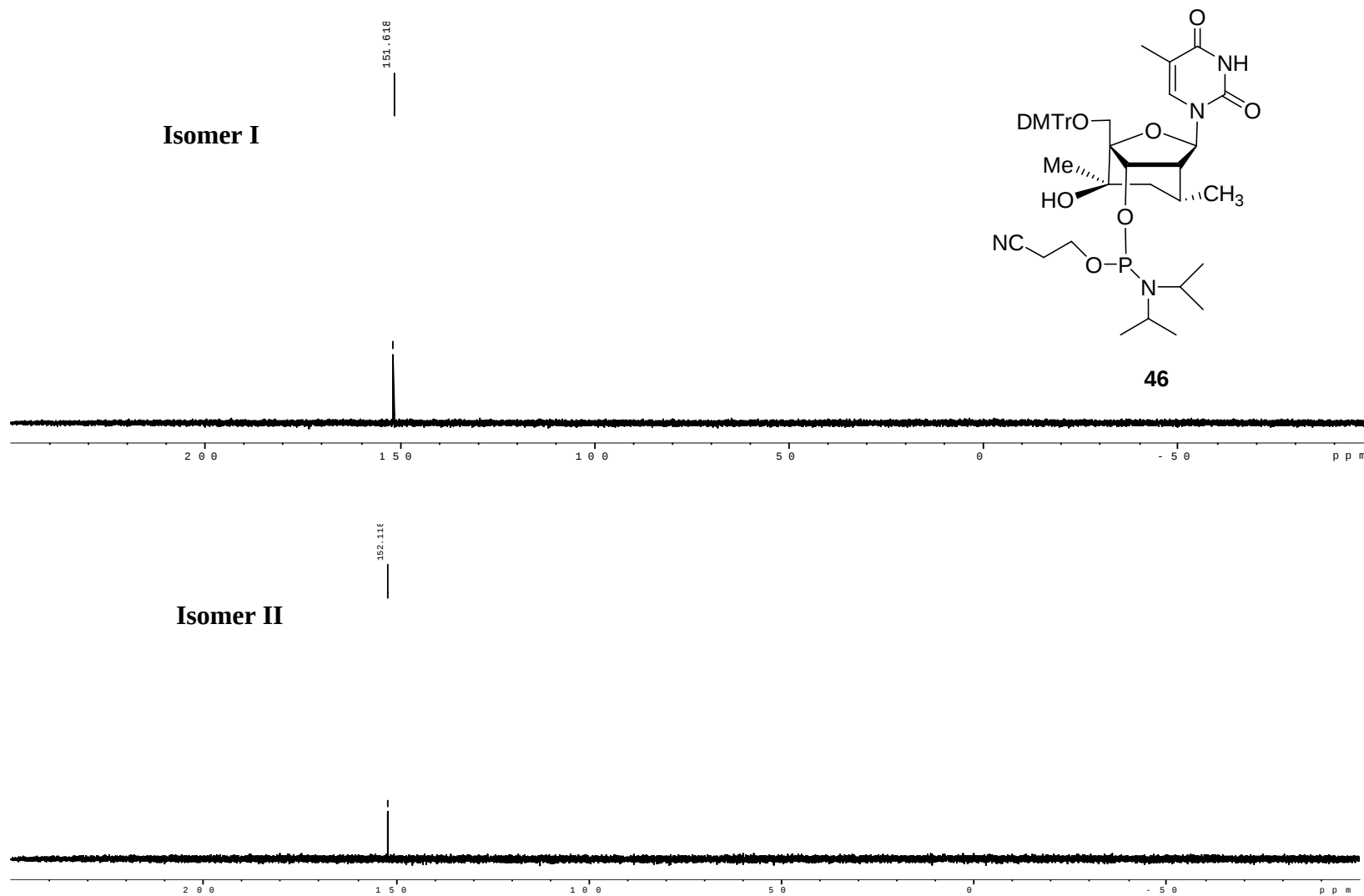


Figure SII.61. ^{31}P NMR spectrum of compound 46.

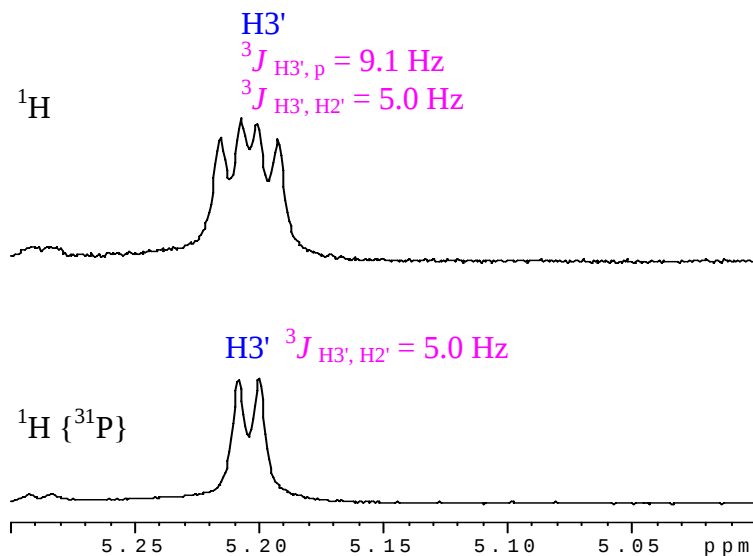


Figure SII.62. ^1H and $^1\text{H} \{^{31}\text{P}\}$ NMR spectrum of compound 46 (isomer I).

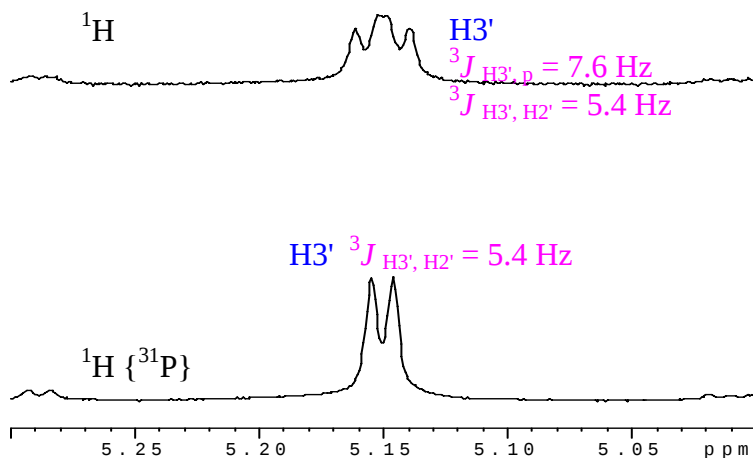
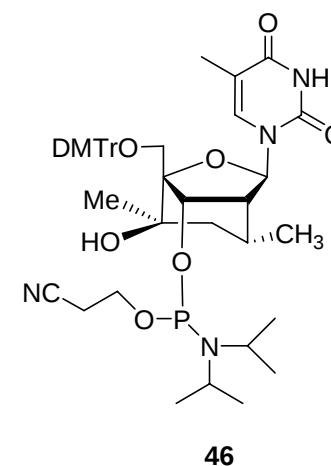


Figure SII.63. ^1H and $^1\text{H} \{^{31}\text{P}\}$ NMR spectrum of compound 46 (isomer II).



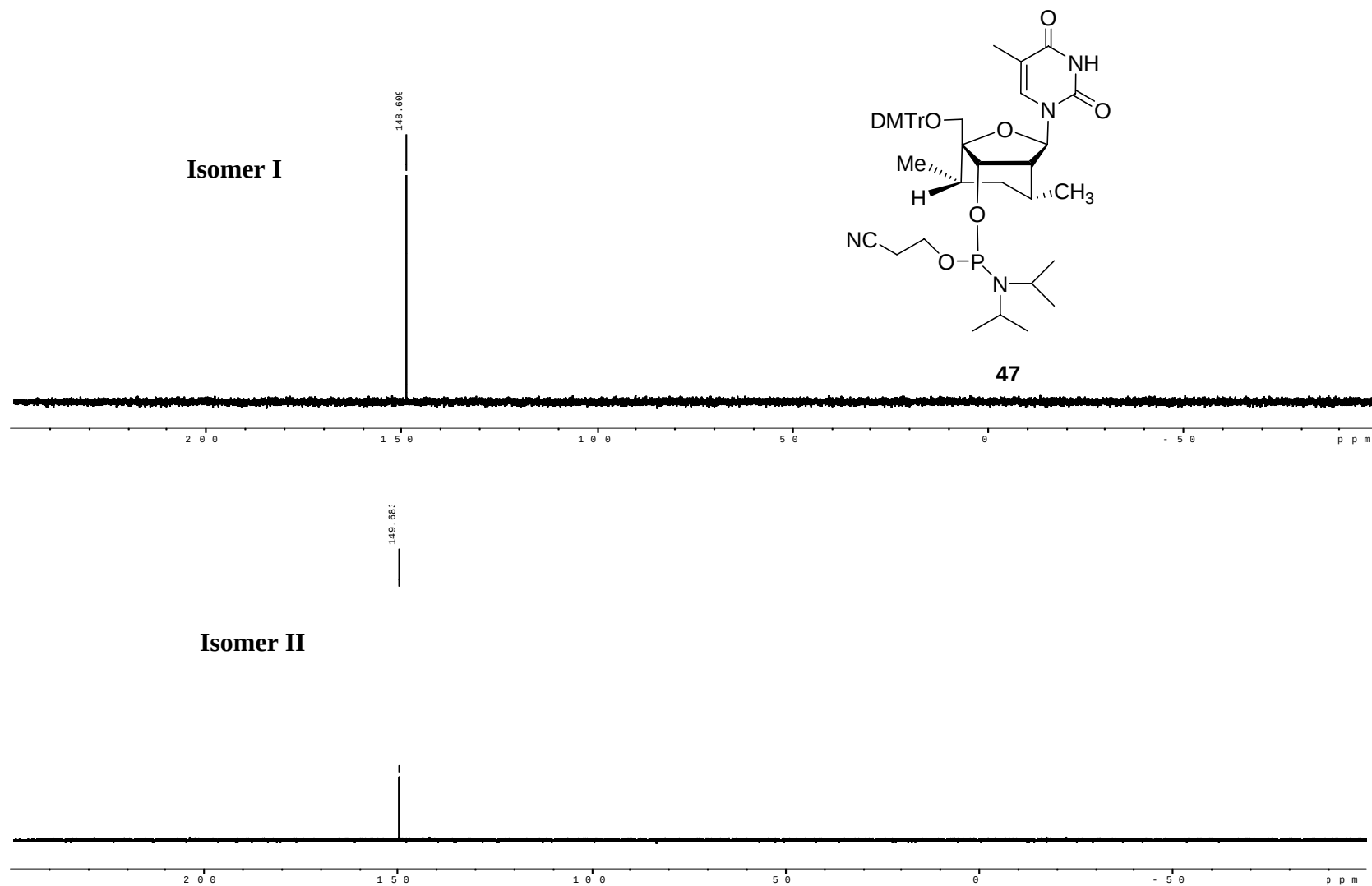


Figure SII.64. ^{31}P NMR spectrum of compound 47.

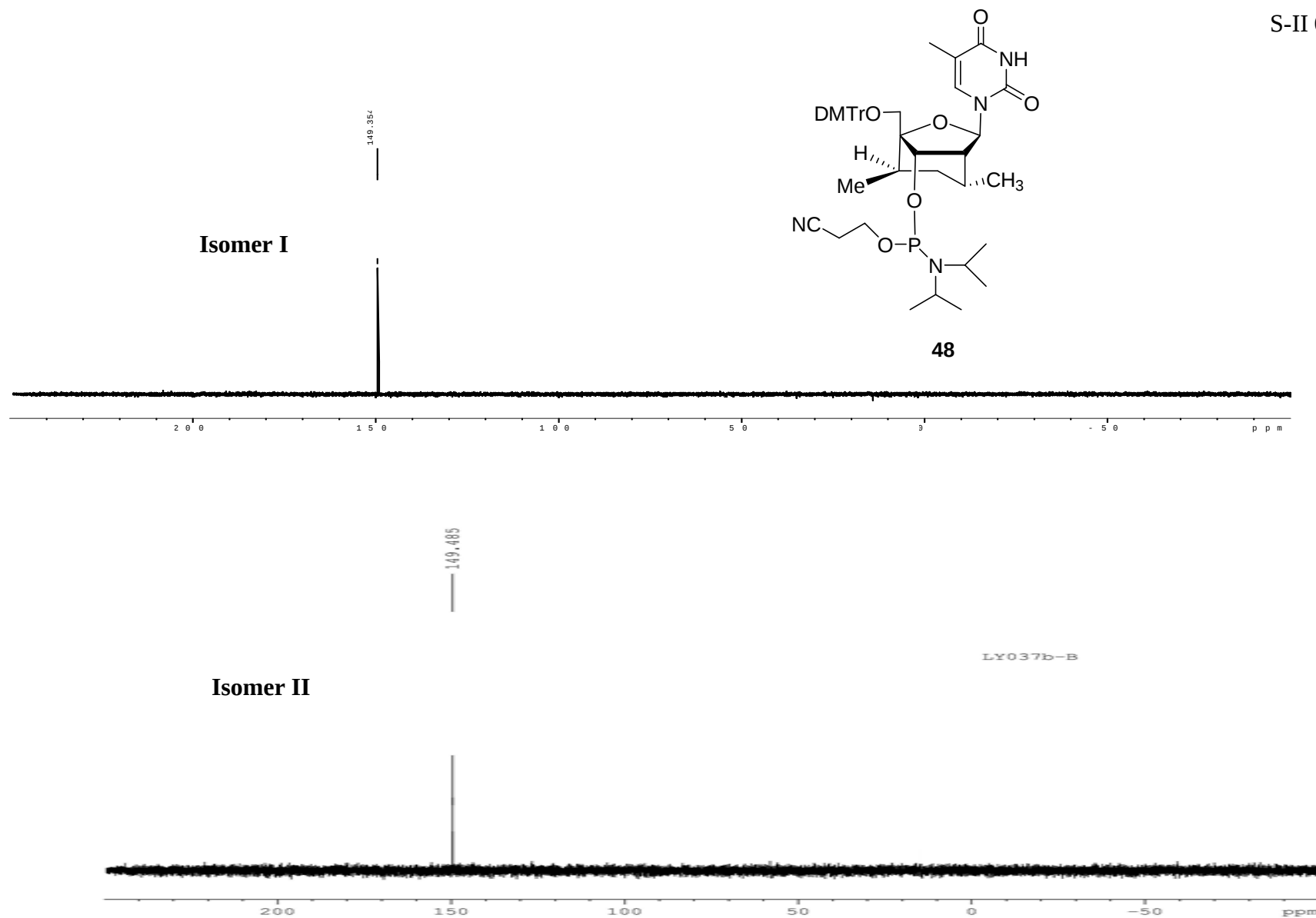


Figure SII.65. ^{31}P NMR spectrum of compound 48.