

Supplementary Materials: Isolation, characterization and antiproliferative activity of new metabolites from the South African endemic red algal species *Laurencia alfredensis*

Godwin A. Dziwornu, Mino R. Caira, Jo-Anne de la Mare, Adrienne L. Edkins, John J. Bolton, Denzil R. Beukes, Suthananda N. Sunassee

Table of Contents:

Scheme S1. Isolation of compounds **1 – 11** from *Laurencia alfredensis*

Figure S1. The structures of compounds **1 – 11** isolated from *Laurencia alfredensis*.

Figure S2. ¹H-NMR spectrum (600MHz, CDCl₃, 303K) of compound **1**

Figure S3. ¹³C-NMR spectrum (150MHz, CDCl₃, 303K) of compound **1**

Figure S4. ¹H-¹H COSY NMR spectrum (600MHz, CDCl₃, 303K) of compound **1**

Figure S5. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compound **1**

Figure S6. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound **1**

Figure S7. ROESY NMR spectrum (600MHz, CDCl₃, 303K) of compound **1**

Figure S8. ¹H NMR spectrum (600MHz, CDCl₃, 303K) of compound **2**

Figure S9. ¹³C NMR spectrum (150MHz, CDCl₃, 303K) of compound **2**

Figure S10. ¹H-¹H COSY NMR spectrum (600MHz, CDCl₃, 303K) of compound **2**

Figure S11. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compound **2**

Figure S12. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound **2**

Figure S13. ROESY NMR spectrum (600MHz, CDCl₃, 303K) of compound **2**

Figure S14. ¹H NMR spectrum (600MHz, CDCl₃, 303K) of compound **3**

Figure S15. ¹³C NMR spectrum (150MHz, CDCl₃, 303K) of compound **3**

Figure S16. ¹H-¹H COSY NMR spectrum (600MHz, CDCl₃, 303K) of compound **3**

Figure S17. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compound **3**

Figure S18. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound **3**

Figure S19. ¹H NMR spectrum (600MHz, CDCl₃, 303K) of compound **4**

Figure S20. ¹³C NMR spectrum (150MHz, CDCl₃, 303K) of compound **4**

Figure S21. ¹H-¹H COSY NMR spectrum (600MHz, CDCl₃, 303K) of compound **4**

Figure S22. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compound **4**

Figure S23. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound **4**

Figure S24. ROESY NMR spectrum (600MHz, CDCl₃, 303K) of compound **4**

Figure S25. ¹H NMR spectrum (600MHz, CDCl₃, 303K) of compounds **5** and **6**

Figure S26. ¹³C NMR spectrum (150MHz, CDCl₃, 303K) of compounds **5** and **6**

Figure S27. ¹H-¹H COSY NMR spectrum (600MHz, CDCl₃, 303K) of compounds **5** and **6**

Figure S28. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compounds **5** and **6**

Figure S29. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compounds **5** and **6**

Figure S30. ROESY NMR spectrum (600MHz, CDCl₃, 303K) of compounds **5** and **6**

Figure S31. ¹H NMR spectrum (600MHz, CDCl₃, 303K) of compound **7**

Figure S32. ¹³C NMR spectrum (150MHz, CDCl₃, 303K) of compound **7**

Figure S33. ¹H-¹H COSY NMR spectrum (600MHz, CDCl₃, 303K) of compound **7**

Figure S34. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compound **7**

Figure S35. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound **7**

Figure S36. ROESY NMR spectrum (600MHz, CDCl₃, 303K) of compound **7**

Figure S37. ¹H NMR spectrum (600MHz, CDCl₃, 303K) of compound **8**

Figure S38. ¹³C NMR spectrum (150MHz, CDCl₃, 303K) of compound **8**

Figure S39. ¹H-¹H COSY NMR spectrum (600MHz, CDCl₃, 303K) of compound **8**

Figure S40. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compound **8**

Figure S41. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound **8**

Figure S42. NOESY NMR spectrum (600MHz, CDCl₃, 303K) of compound **8**

Figure S43. ¹H-NMR spectrum (600MHz, CDCl₃, 303K) of compound **9**

Figure S44. ¹³C-NMR spectrum (150MHz, CDCl₃, 303K) of compound **9**

Figure S45. ¹H-¹H COSY NMR spectrum (600MHz, CDCl₃, 303K) of compound **9**

Figure S46. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compound **9**

Figure S47. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound **9**

Figure S48. ROESY NMR spectrum (600MHz, CDCl₃, 303K) of compound **9**

Figure S49. ¹H-NMR spectrum (600MHz, CDCl₃, 303K) of compound **10**

Figure S50. ¹³C-NMR spectrum (150MHz, CDCl₃, 303K) of compound **10**

Figure S51. ^1H - ^1H COSY NMR spectrum (600MHz, CDCl_3 , 303K) of compound **10**

Figure S52. HSQC-DEPT NMR spectrum (600MHz, CDCl_3 , 303K) of compound **10**

Figure S53. HMBC NMR spectrum (600MHz, CDCl_3 , 303K) of compound **10**

Figure S54. ROESY NMR spectrum (600MHz, CDCl_3 , 303K) of compound **10**

Figure S55. ^1H -NMR spectrum (600MHz, DMSO-d_6 , 303K) of compound **11**

Figure S56. ^{13}C -NMR spectrum (150MHz, DMSO-d_6 , 303K) of compound **11**

Figure S57. ^1H - ^1H COSY NMR spectrum (600MHz, DMSO-d_6 , 303K) of compound **11**

Figure S58. HSQC-DEPT NMR spectrum (600MHz, DMSO-d_6 , 303K) of compound **11**

Figure S59. HMBC NMR spectrum (600MHz, DMSO-d_6 , 303K) of compound **11**

Figure S60. HR-ESI-MS spectrum of compound **1**

Figure S61. HR-ESI-MS spectrum of compound **2**

Figure S62. HR-ESI-MS spectrum of compound **3**

Figure S63. HR-ESI-MS spectrum of compound **5**

Figure S64. HR-ESI-MS spectrum of compound **6**

Figure S65. HR-ESI-MS spectrum of compound **7**

Figure S66. HR-ESI-MS spectrum of compound **8**

Figure S67. HR-ESI-MS spectrum of compound **9**

Figure S68. HR-ESI-MS spectrum of compound **10**

Figure S69. HR-ESI-MS spectrum of compound **11**

Figure S70. IR spectrum of compound **1**

Figure S71. IR spectrum of compound **2**

Figure S72. IR spectrum of compound **3**

Figure S73. IR spectrum of compound **7**

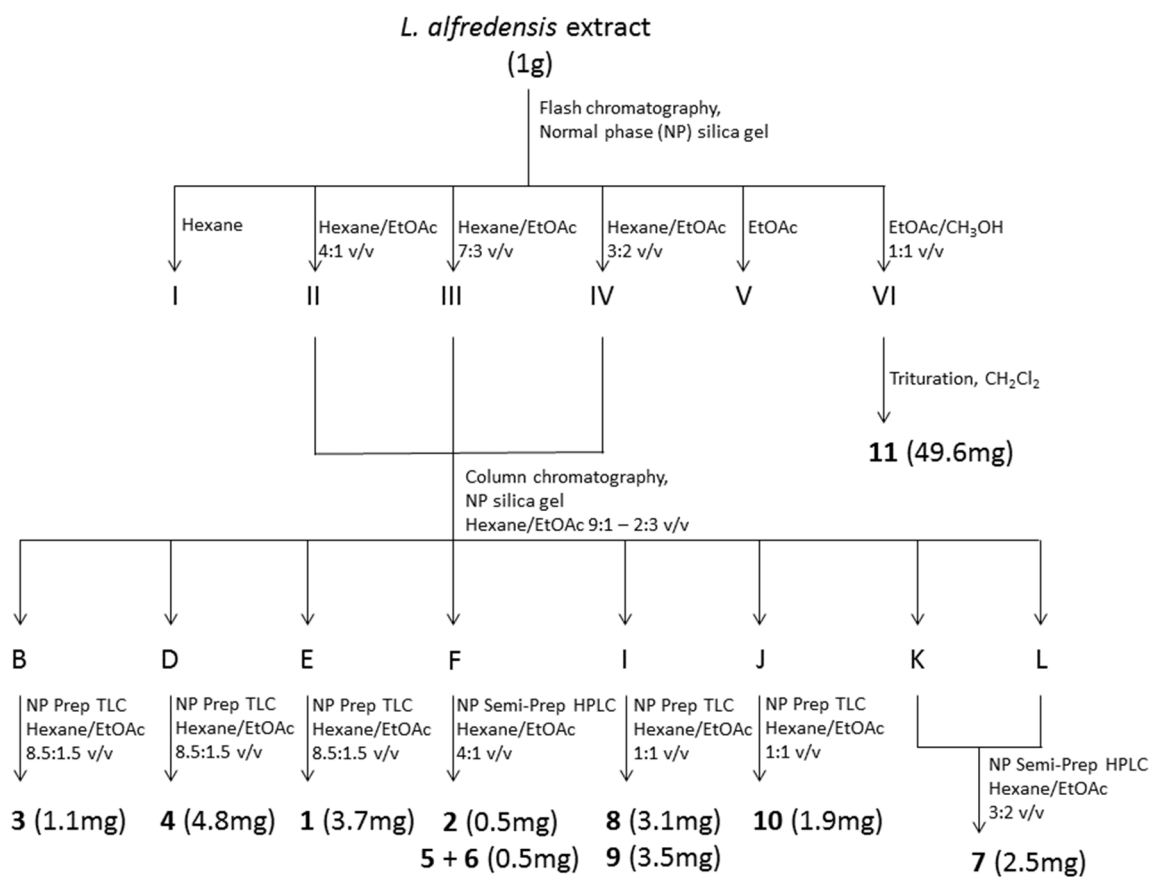
Figure S74. IR spectrum of compound **8**

Figure S75. IR spectrum of compound **10**

Figure S76. UV spectrum of compound **8**

Figure S77. UV spectrum of compound **10**

Table S1. Cytotoxicity assay data for compounds **1 - 10**



Scheme S1. Isolation of compounds **1 – 11** from *Laurencia alfredensis*

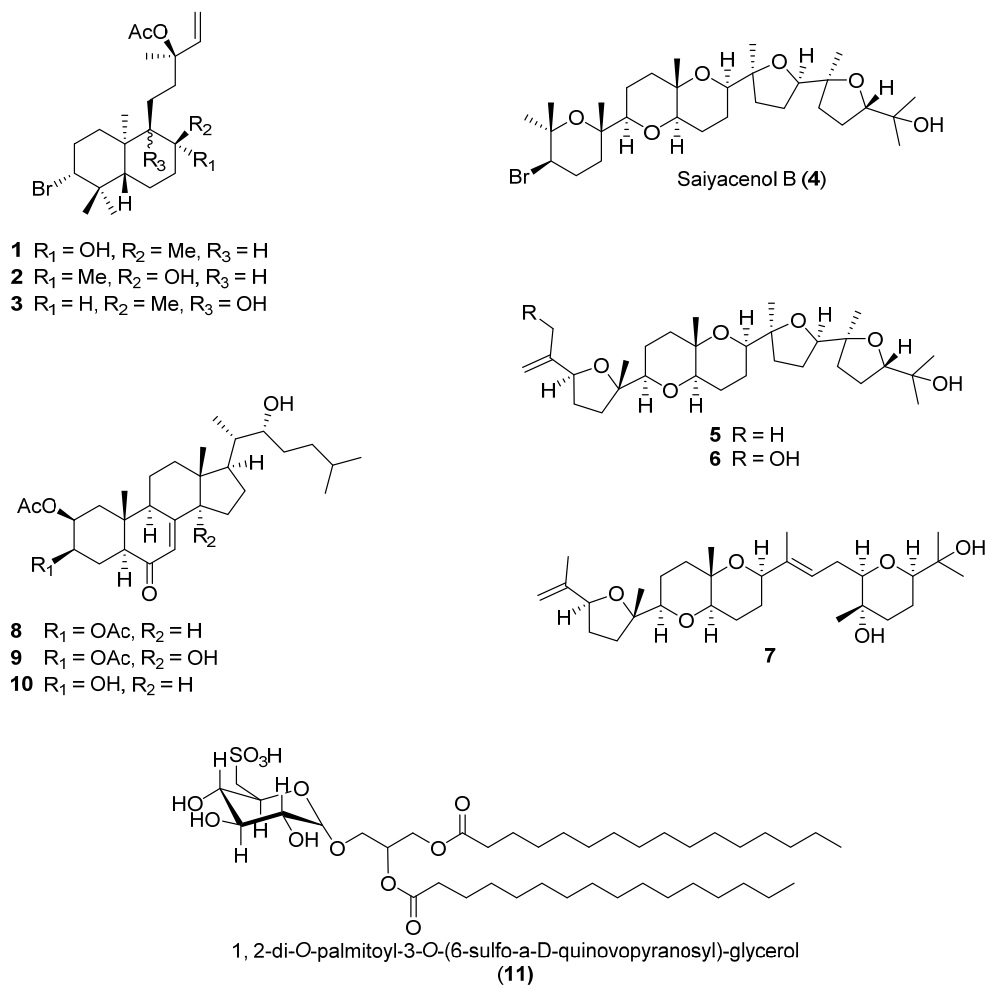


Figure S1. The structures of compounds **1** – **11** isolated from *Laurencia alfredensis*.

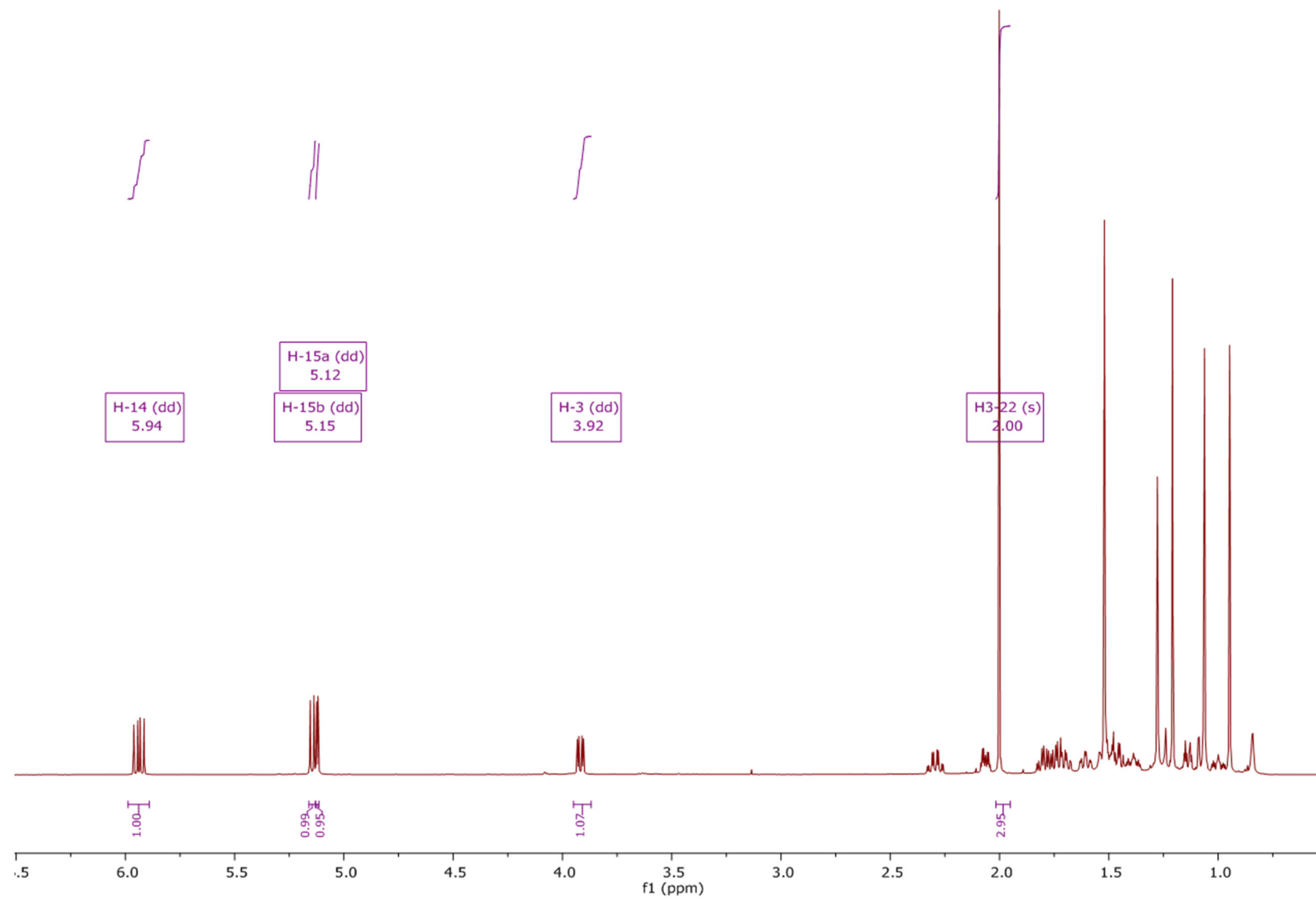


Figure S2. ¹H-NMR spectrum (600MHz, CDCl₃, 303K) of compound **1**

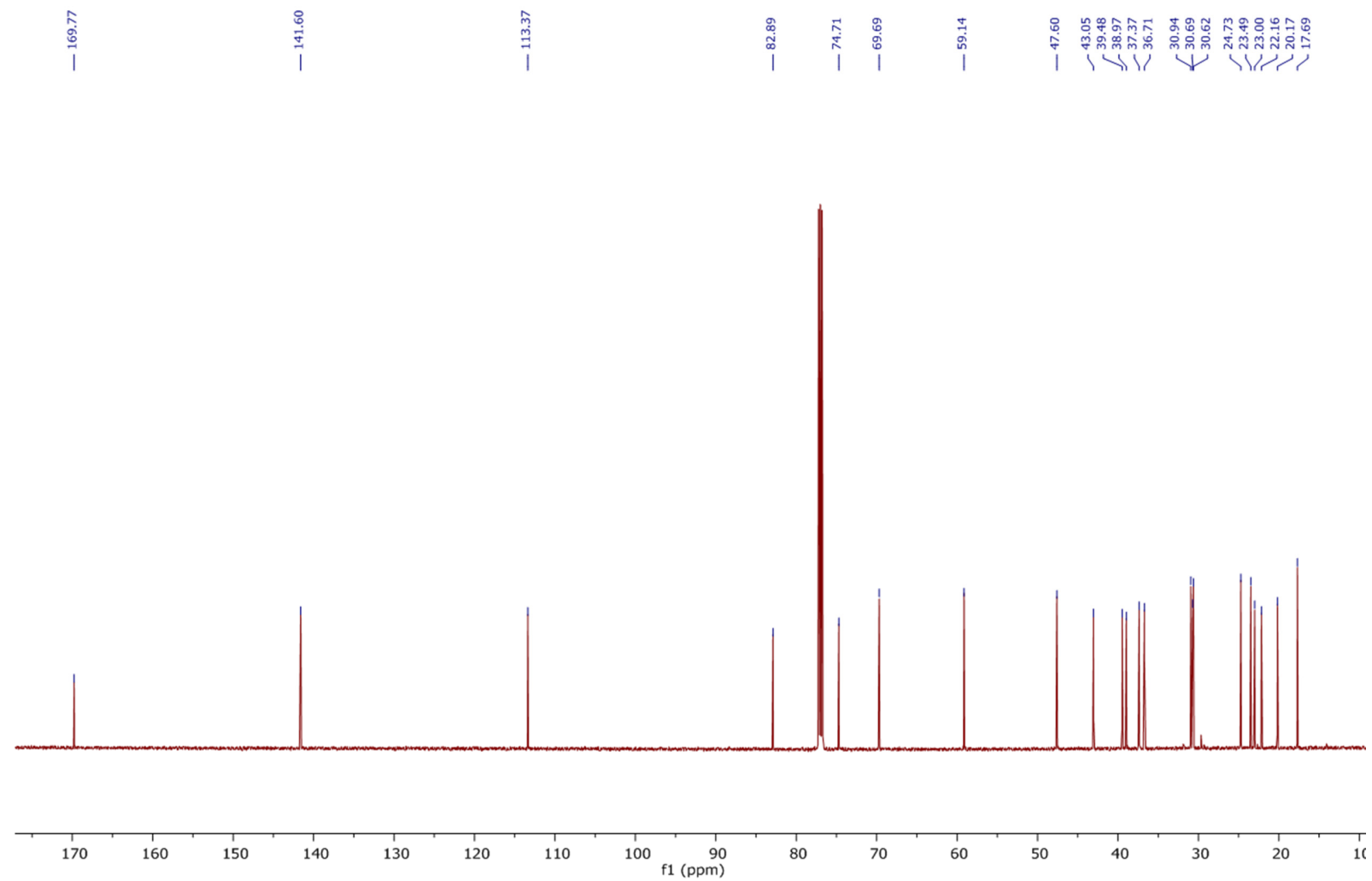


Figure S3. ^{13}C -NMR spectrum (150MHz, CDCl_3 , 303K) of compound 1

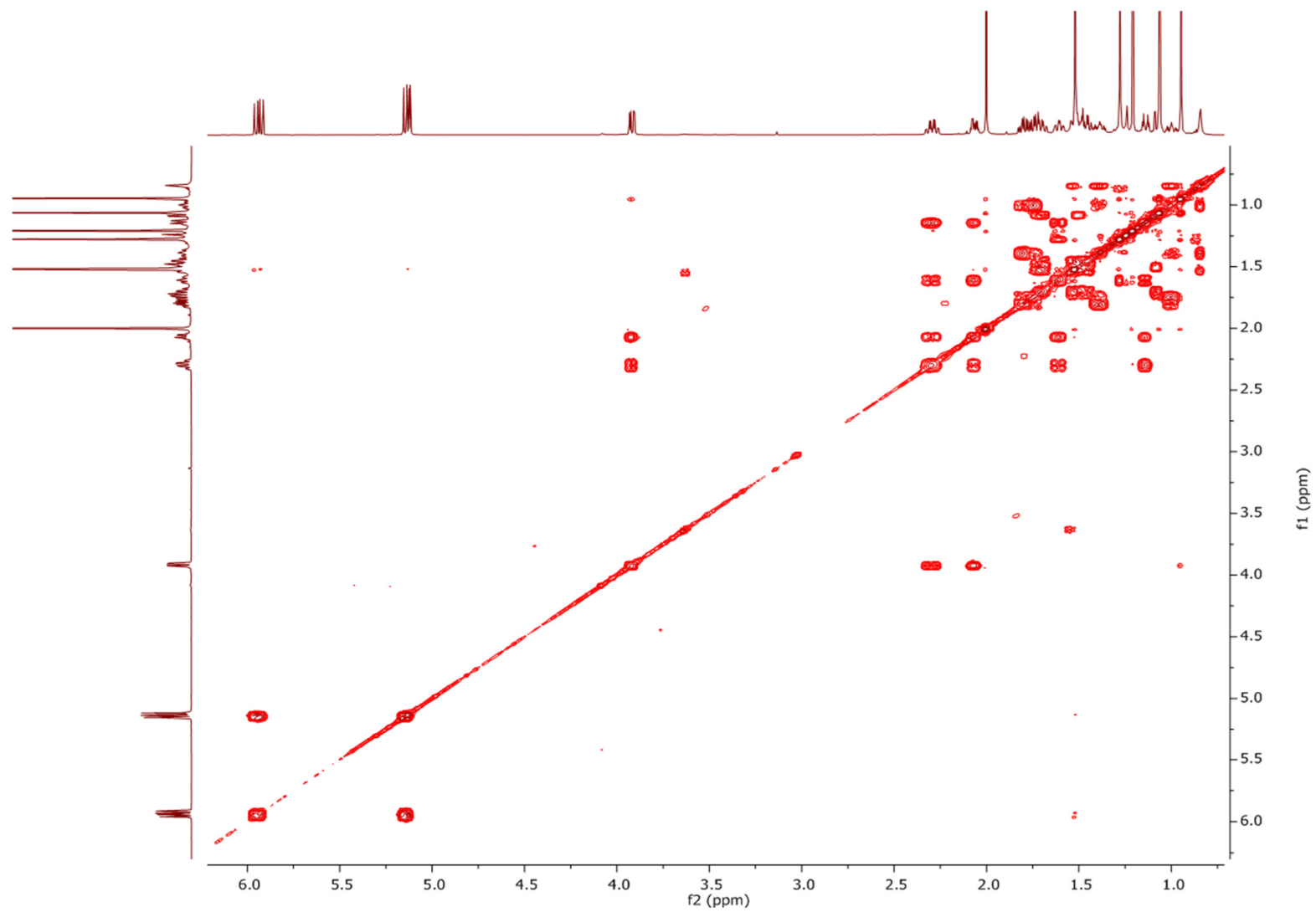


Figure S4. ^1H - ^1H COSY spectrum (600MHz, CDCl_3 , 303K) of compound **1**

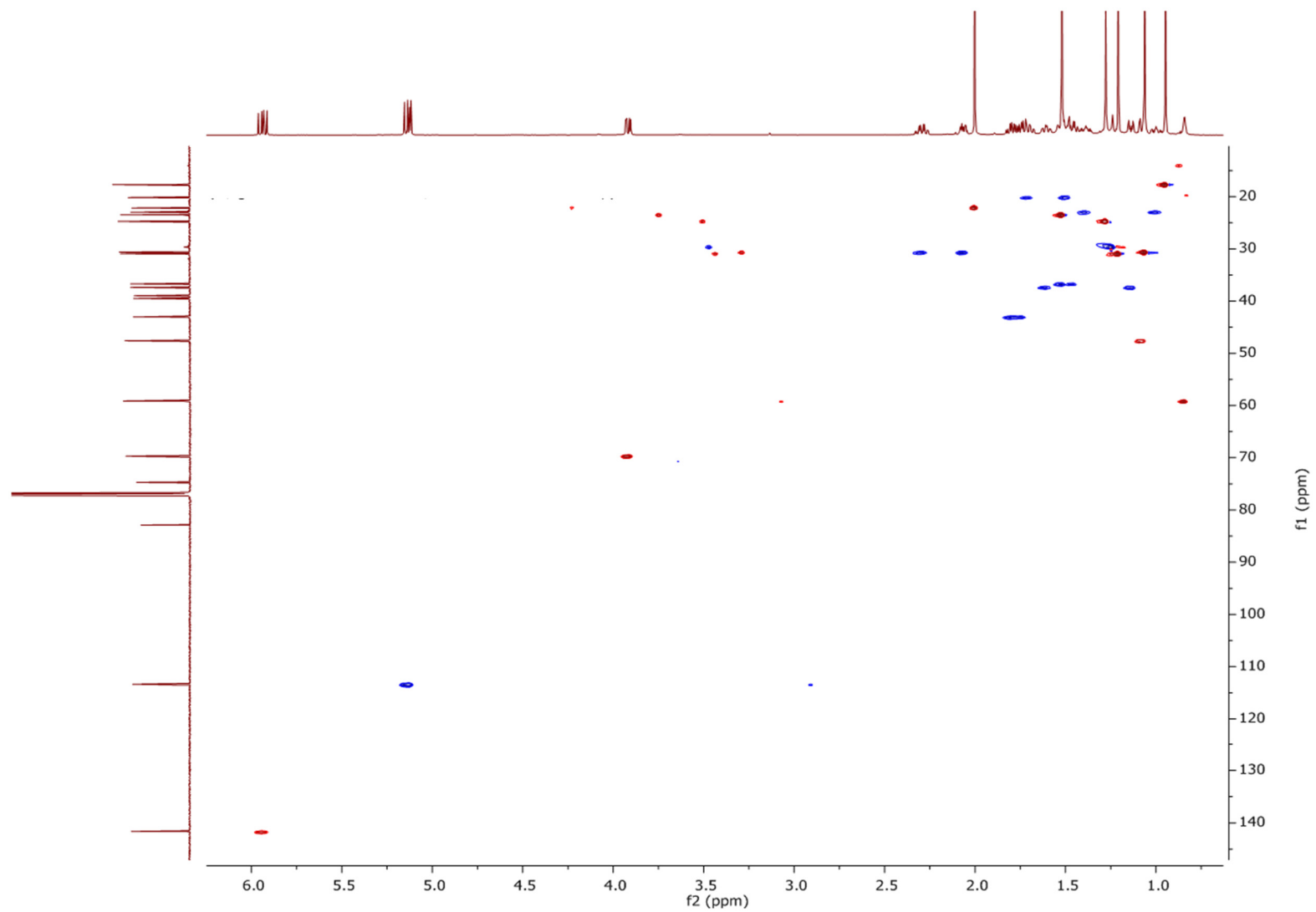


Figure S5. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compound **1**

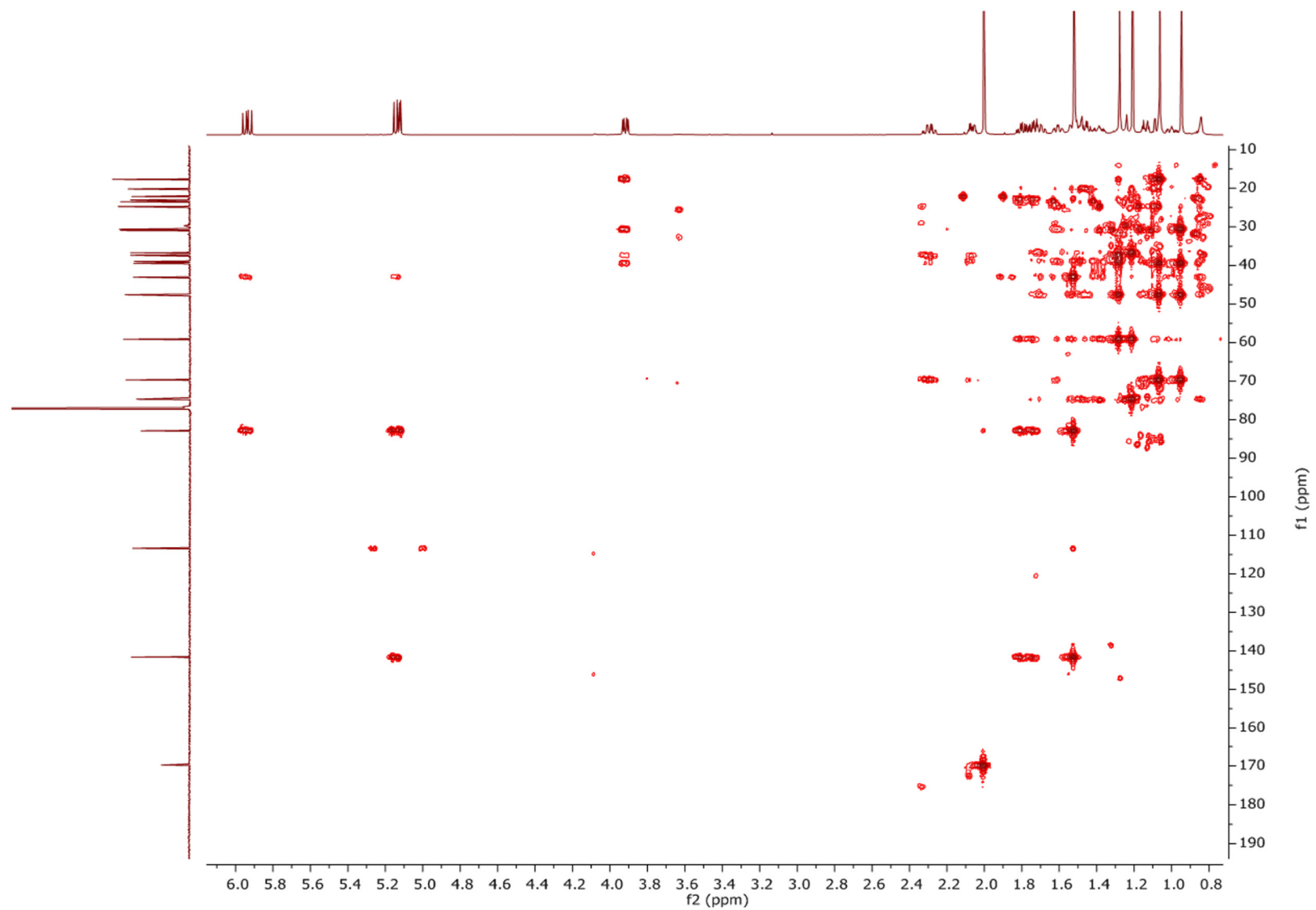


Figure S6. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound **1**

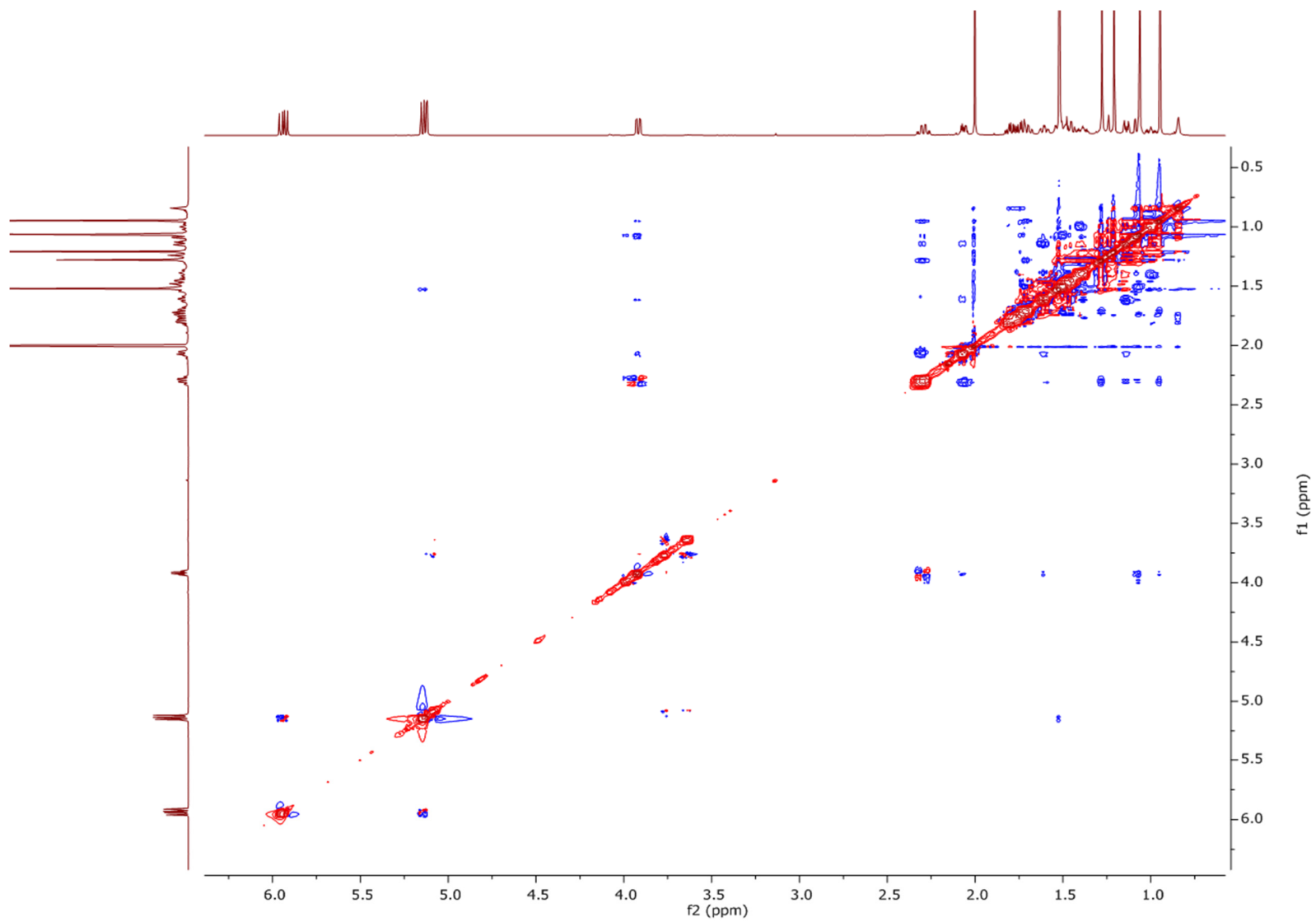


Figure S7. ROESY NMR spectrum (600MHz, CDCl₃, 303K) of compound **1**

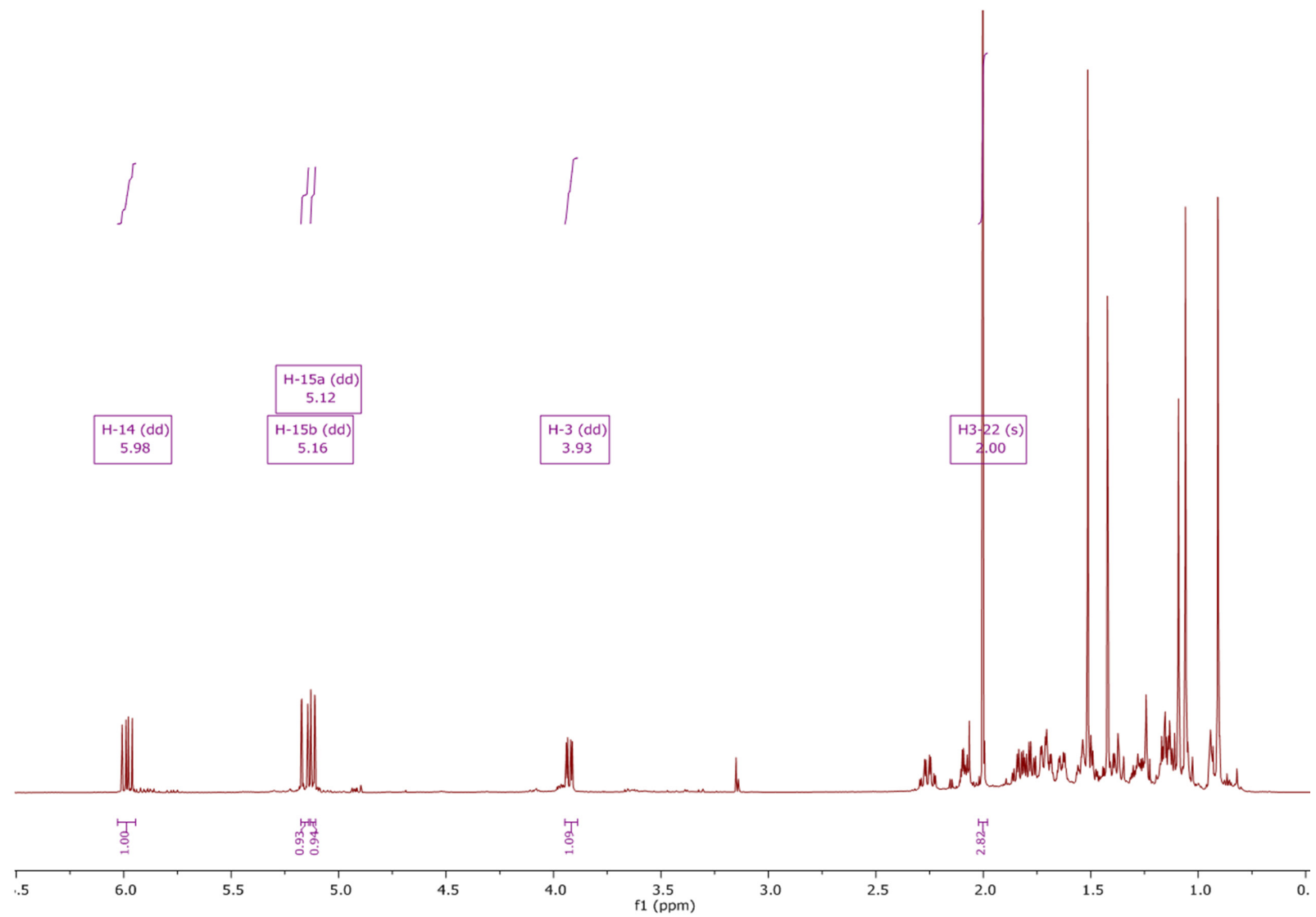


Figure S8. ¹H-NMR spectrum (600MHz, CDCl₃, 303K) of compound 2

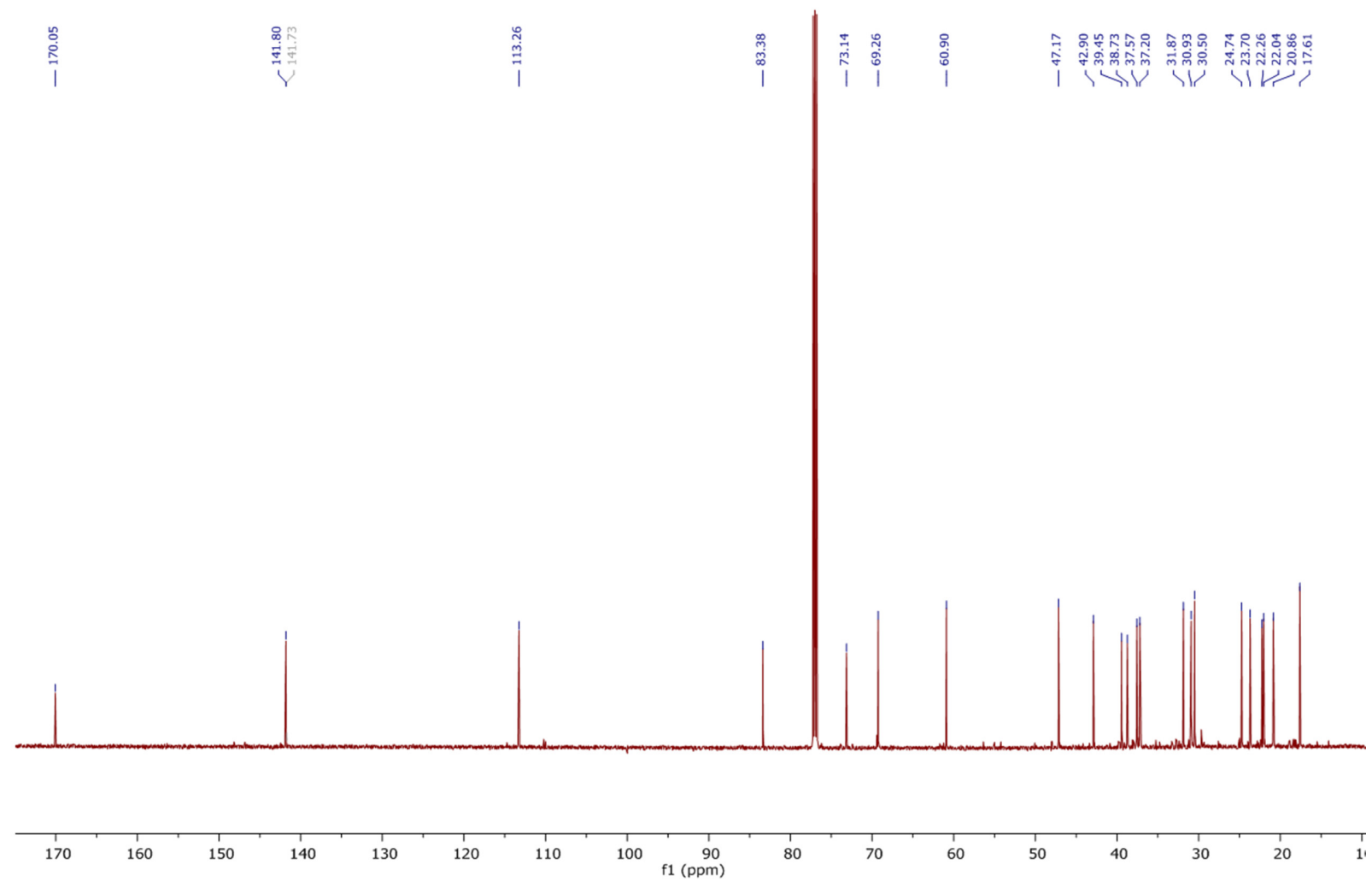


Figure S9. ^{13}C -NMR spectrum (150MHz, CDCl_3 , 303K) of compound 2

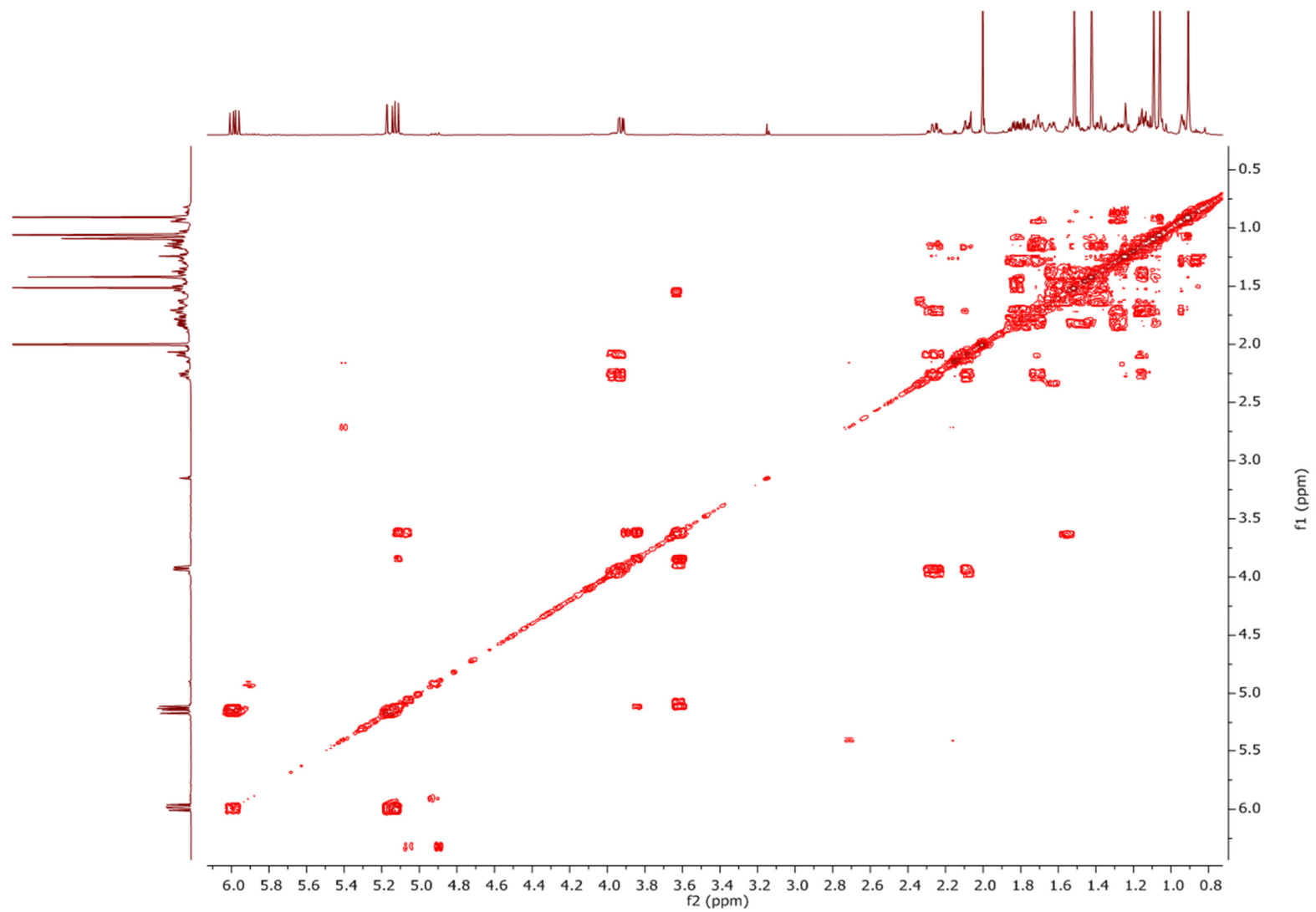


Figure S10. ^1H - ^1H COSY NMR spectrum (600MHz, CDCl_3), 303K of compound **2**

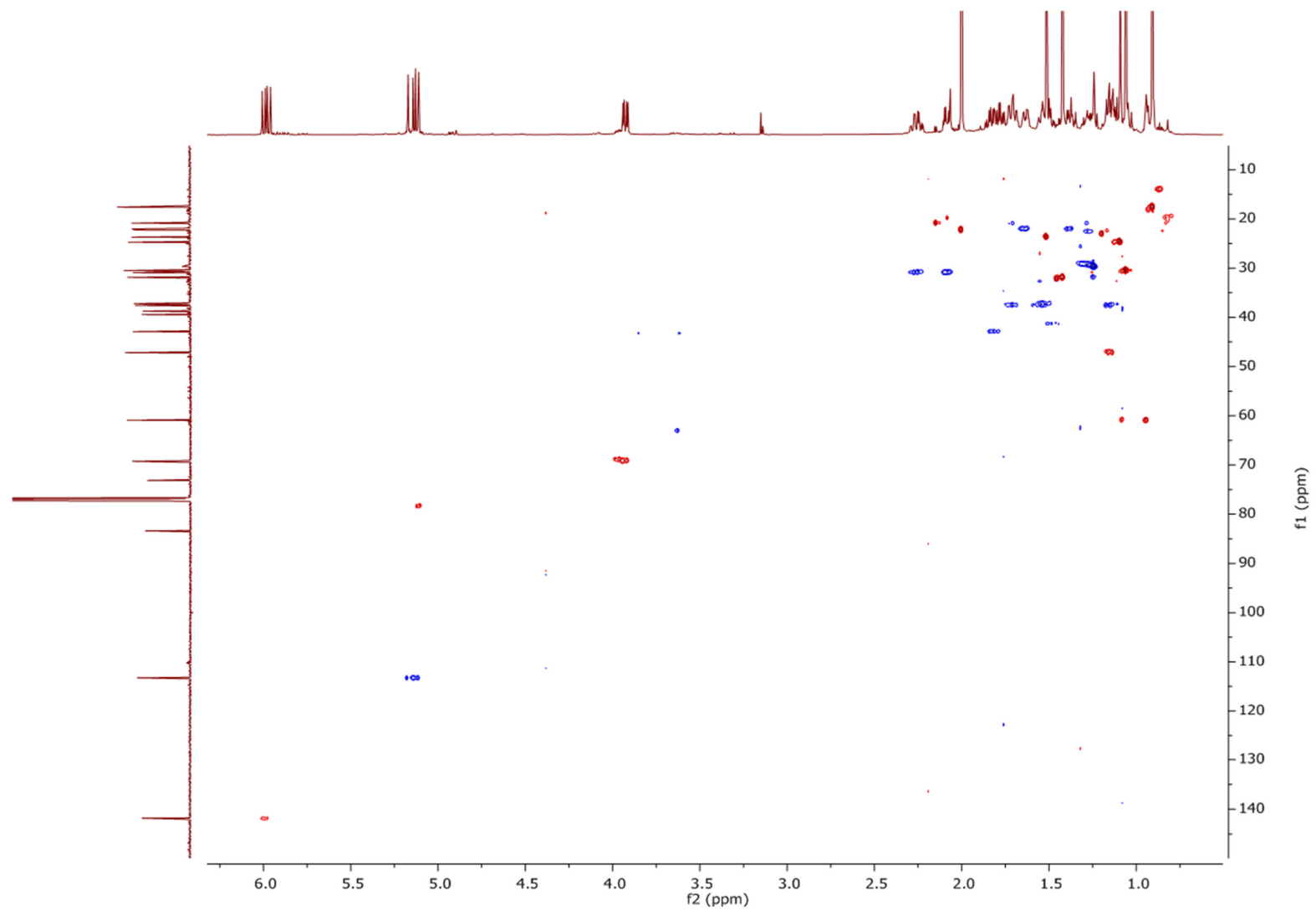


Figure S11. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compound **2**

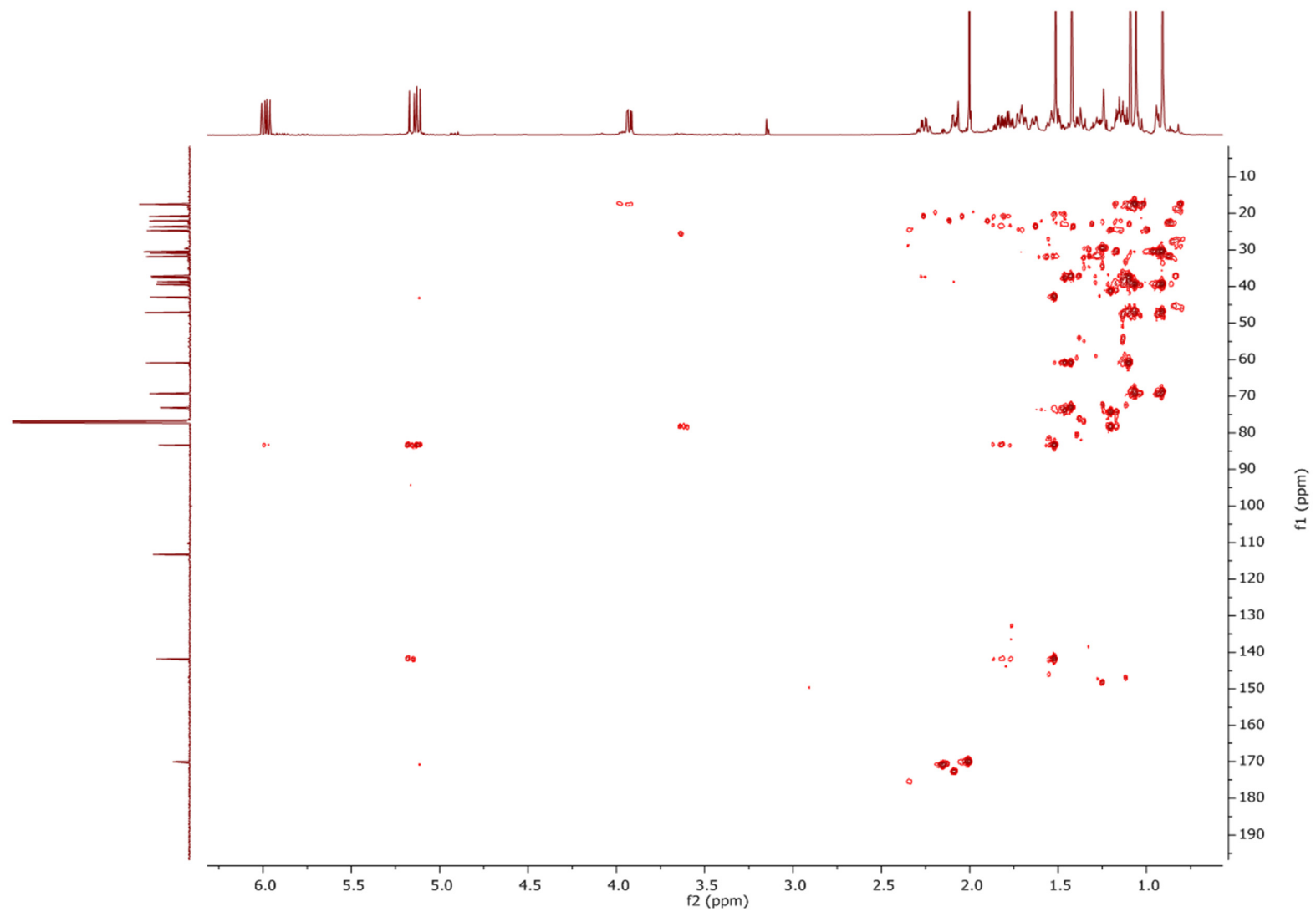


Figure S12. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound **2**

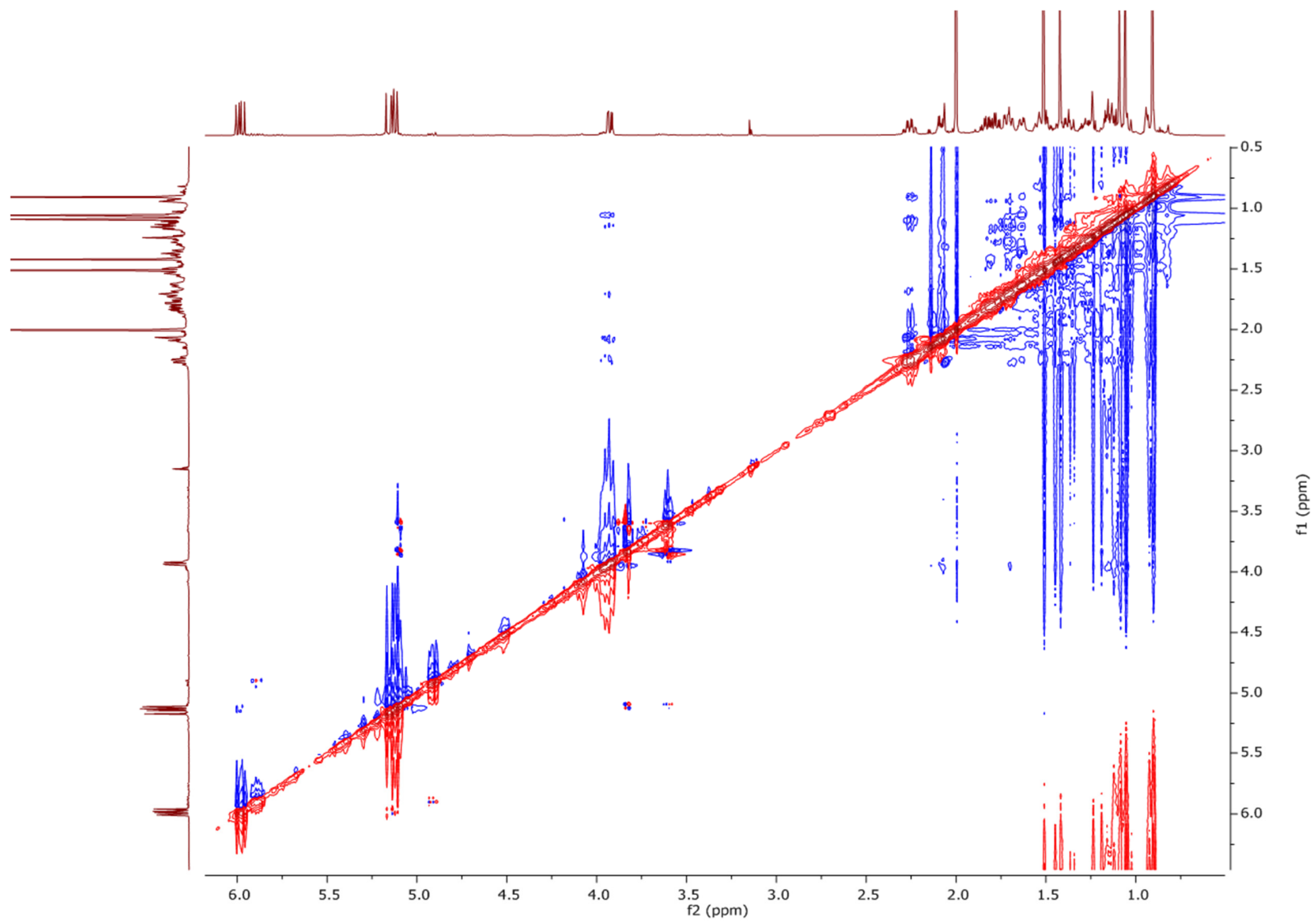


Figure S13. ROESY NMR spectrum (600MHz, CDCl₃, 303K) of compound **2**

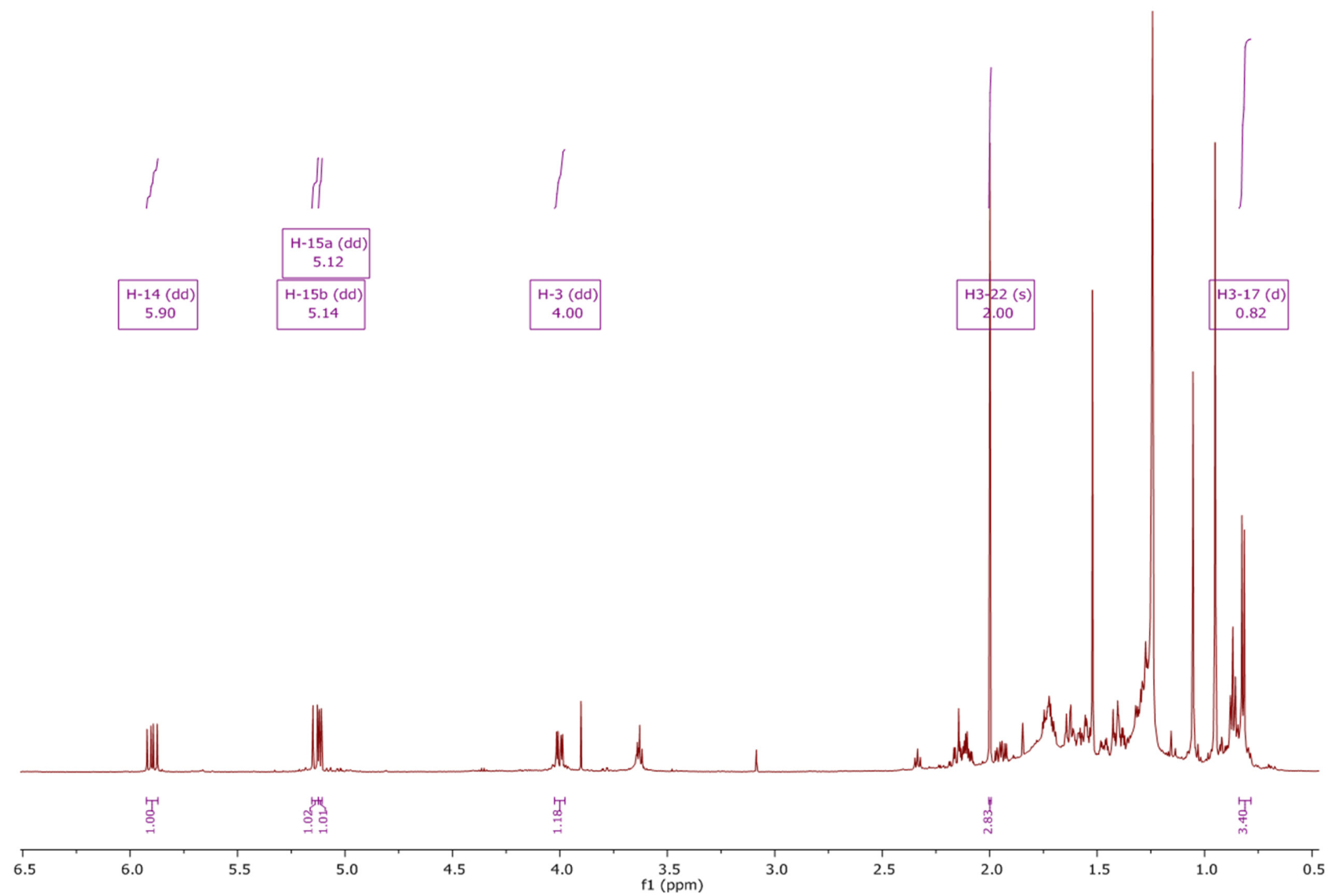


Figure S14. ¹H-NMR spectrum (600MHz, CDCl₃, 303K) of compound 3

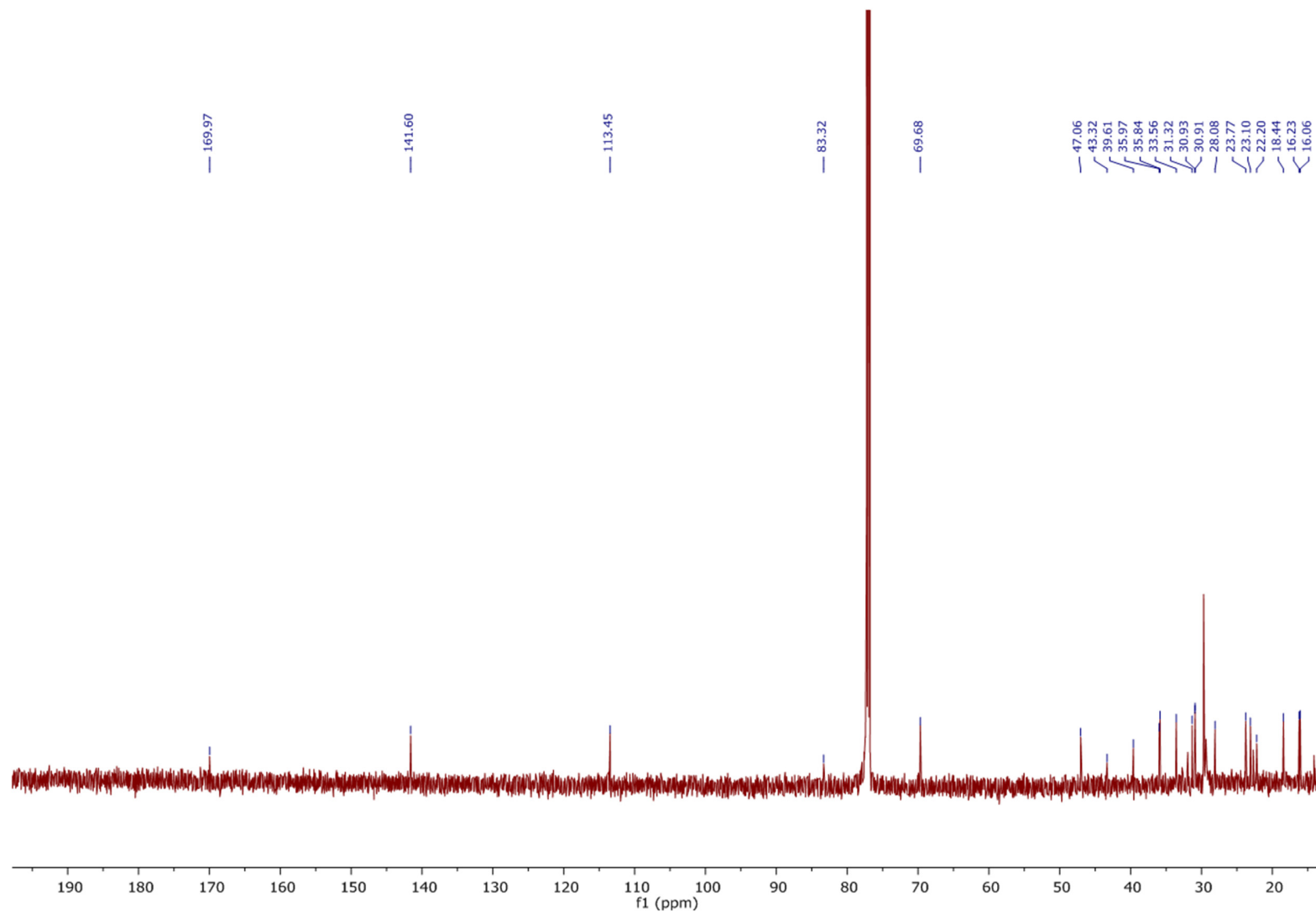


Figure S15. ^{13}C -NMR spectrum (150MHz, CDCl_3 , 303K) of compound 3

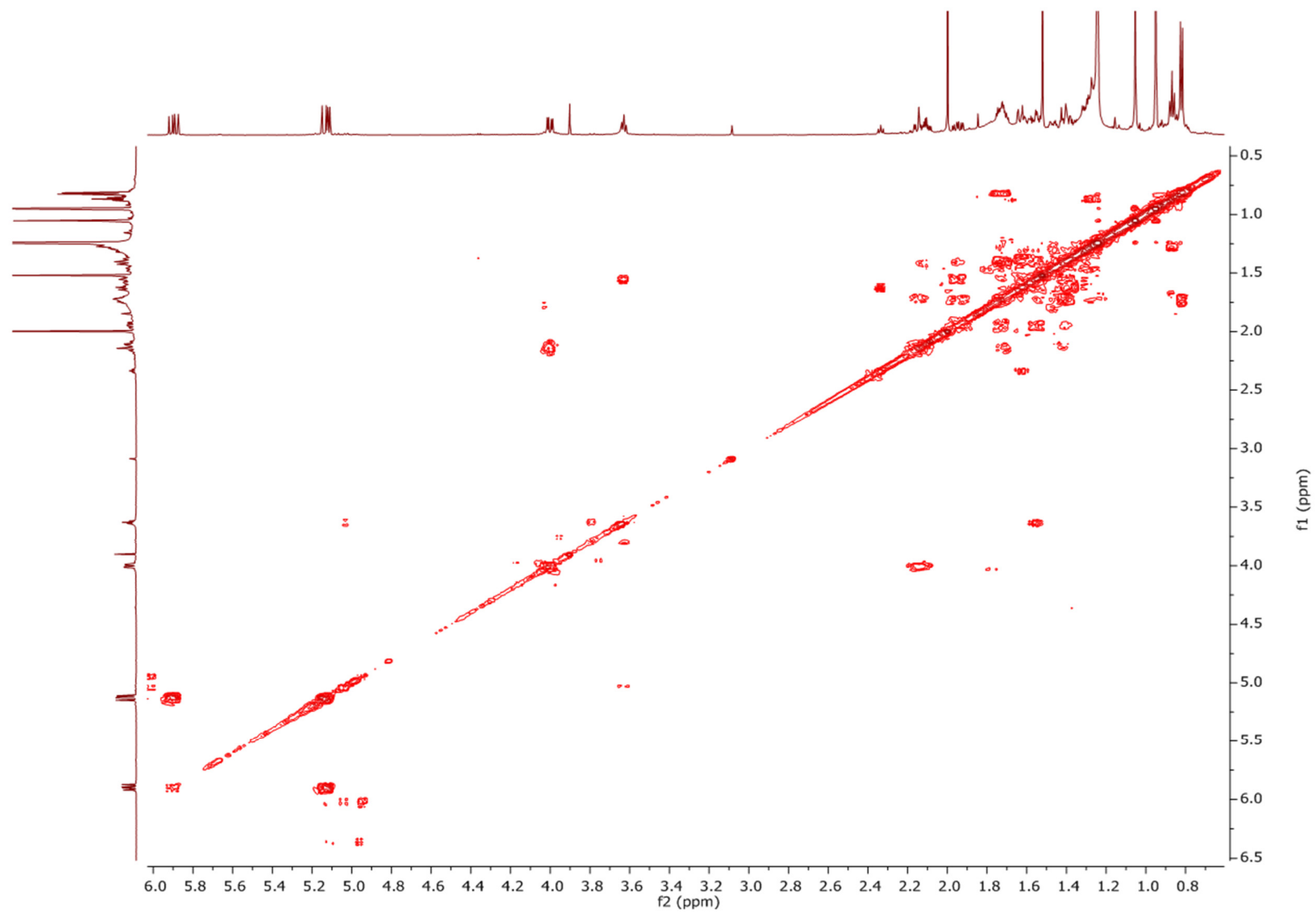


Figure S16. ^1H - ^1H COSY NMR spectrum (600MHz, CDCl_3 , 303K) of compound **3**

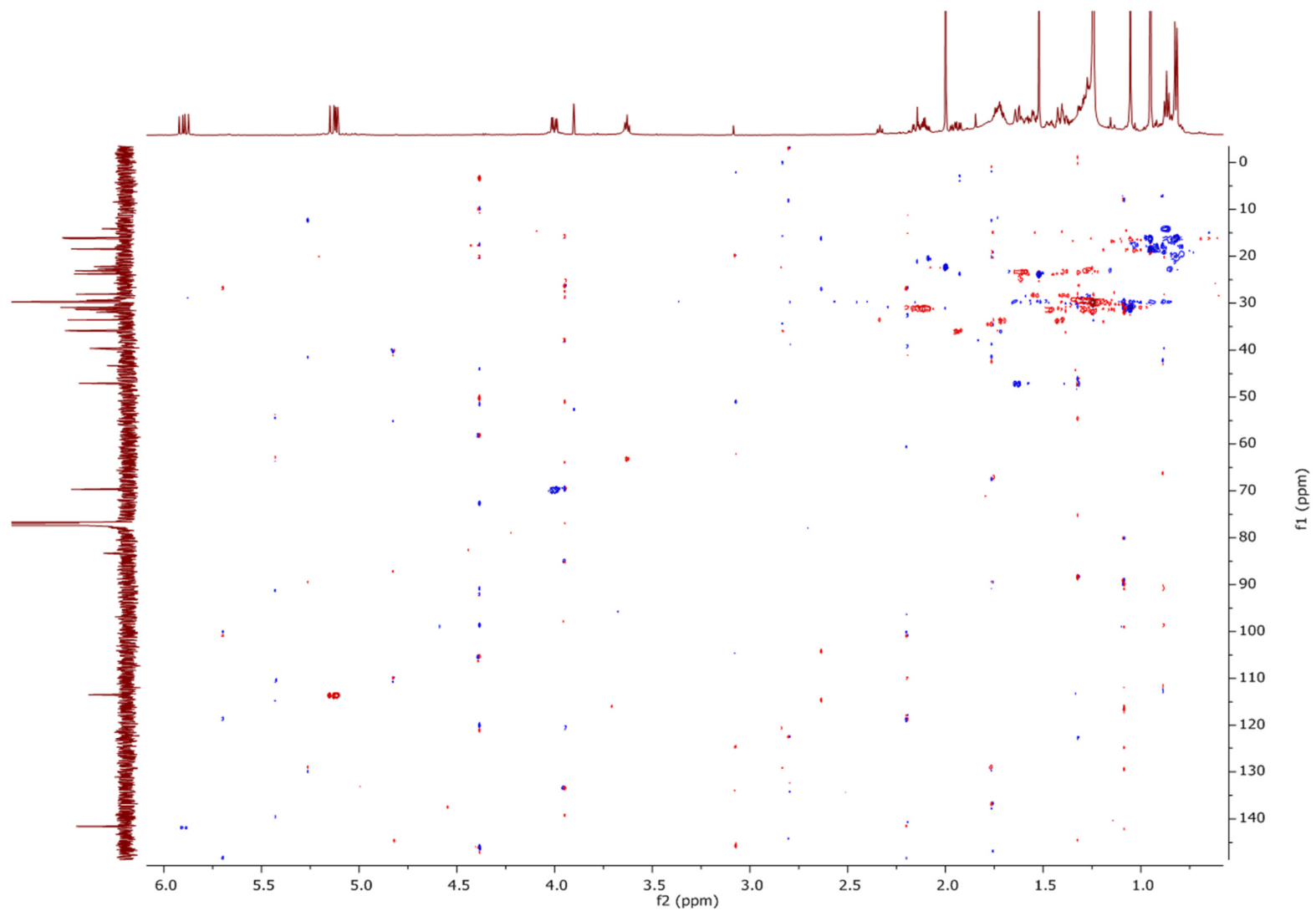


Figure S17. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compound 3

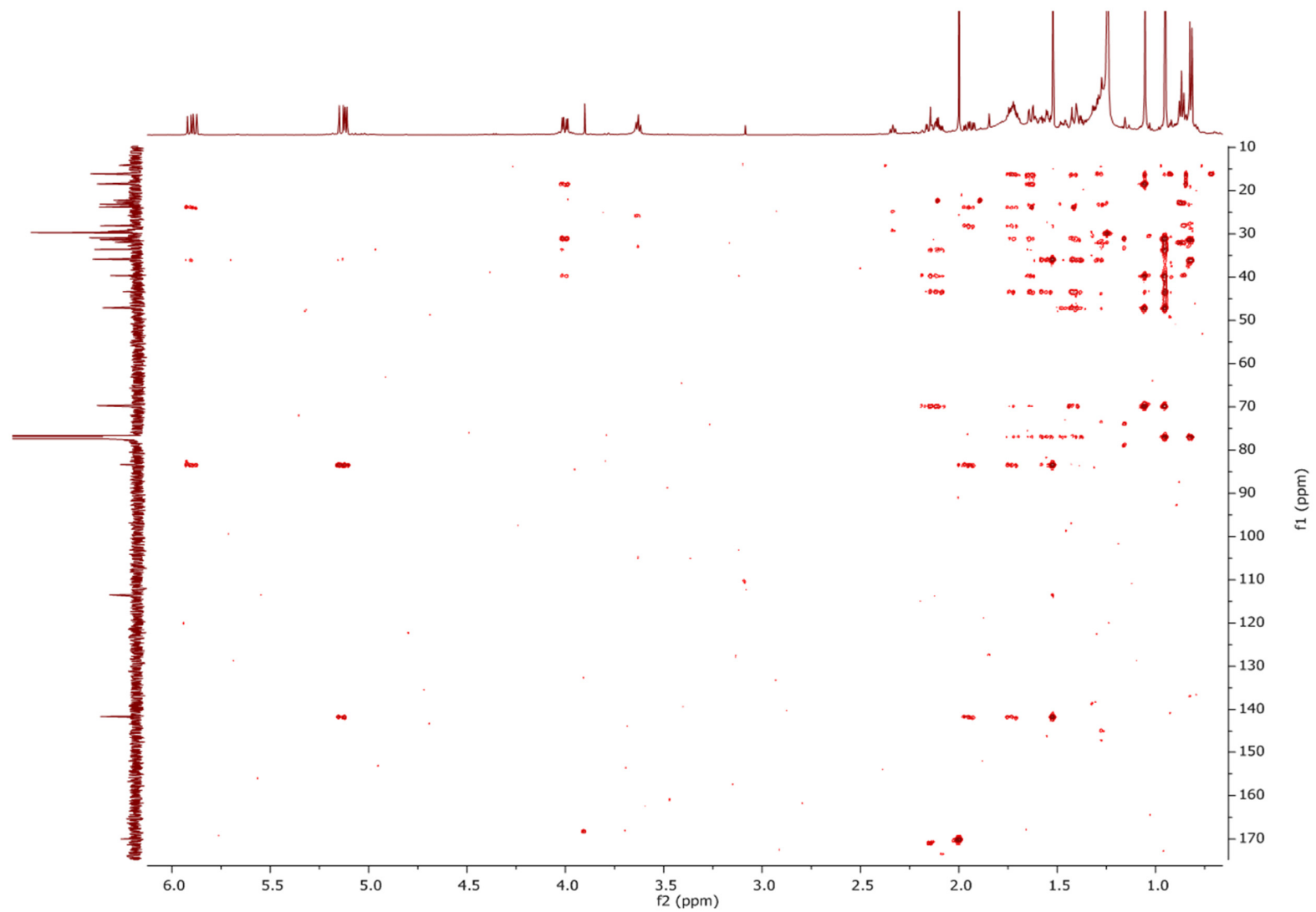


Figure S18. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound **3**

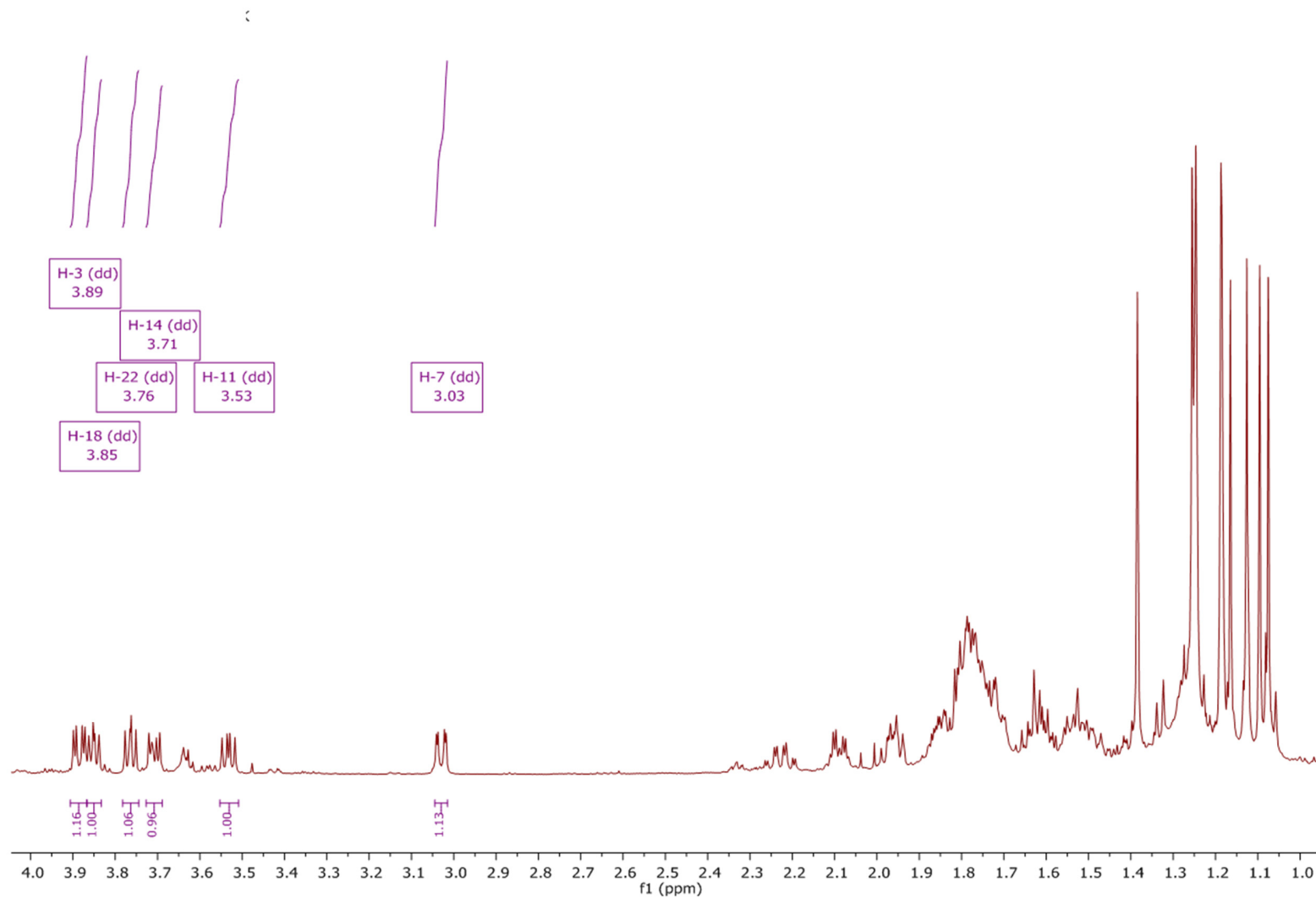


Figure S19. ¹H-NMR spectrum (600MHz, CDCl₃, 303K) of compound 4

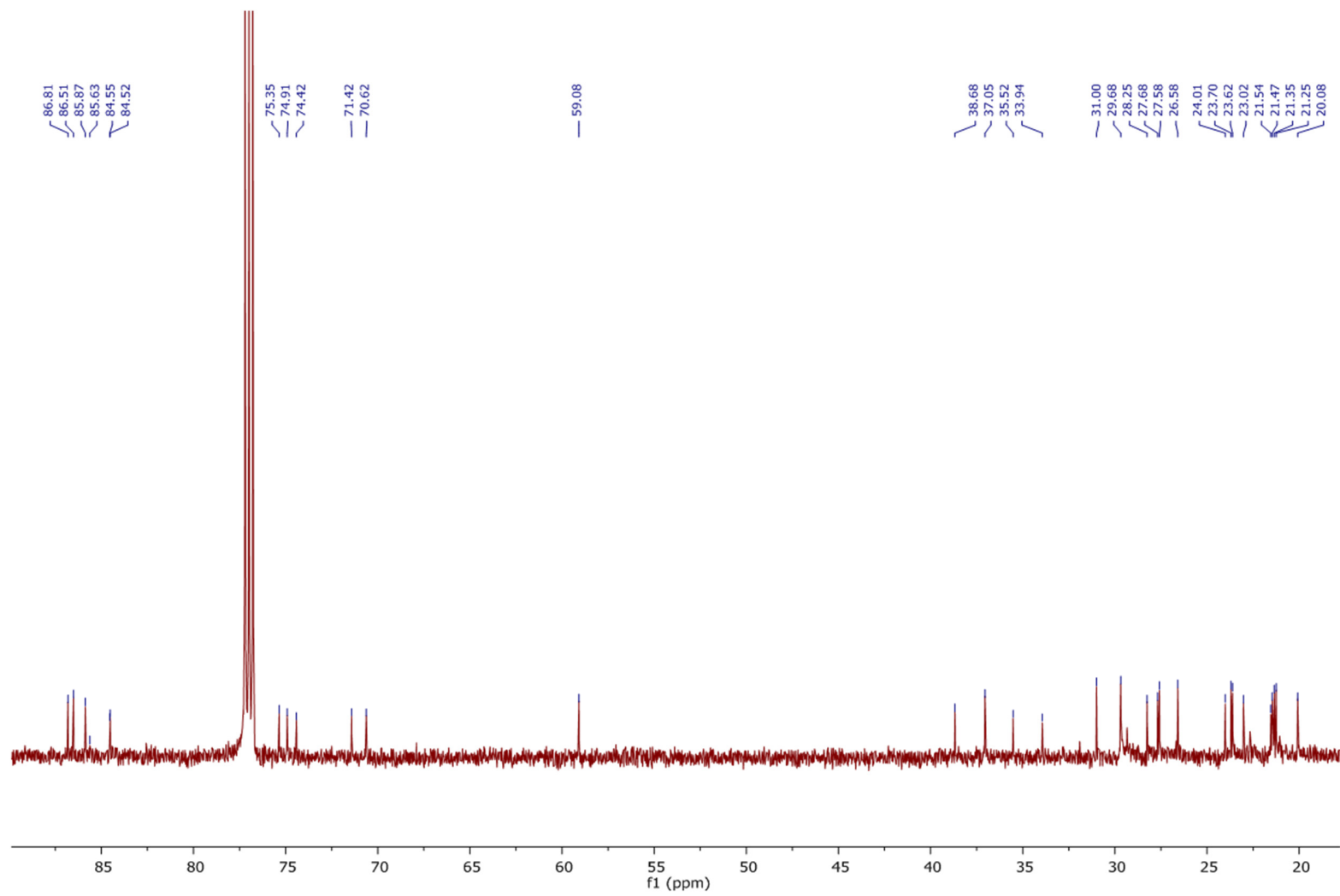


Figure S20. ^{13}C -NMR spectrum (150MHz, CDCl_3 , 303K) of compound **4**

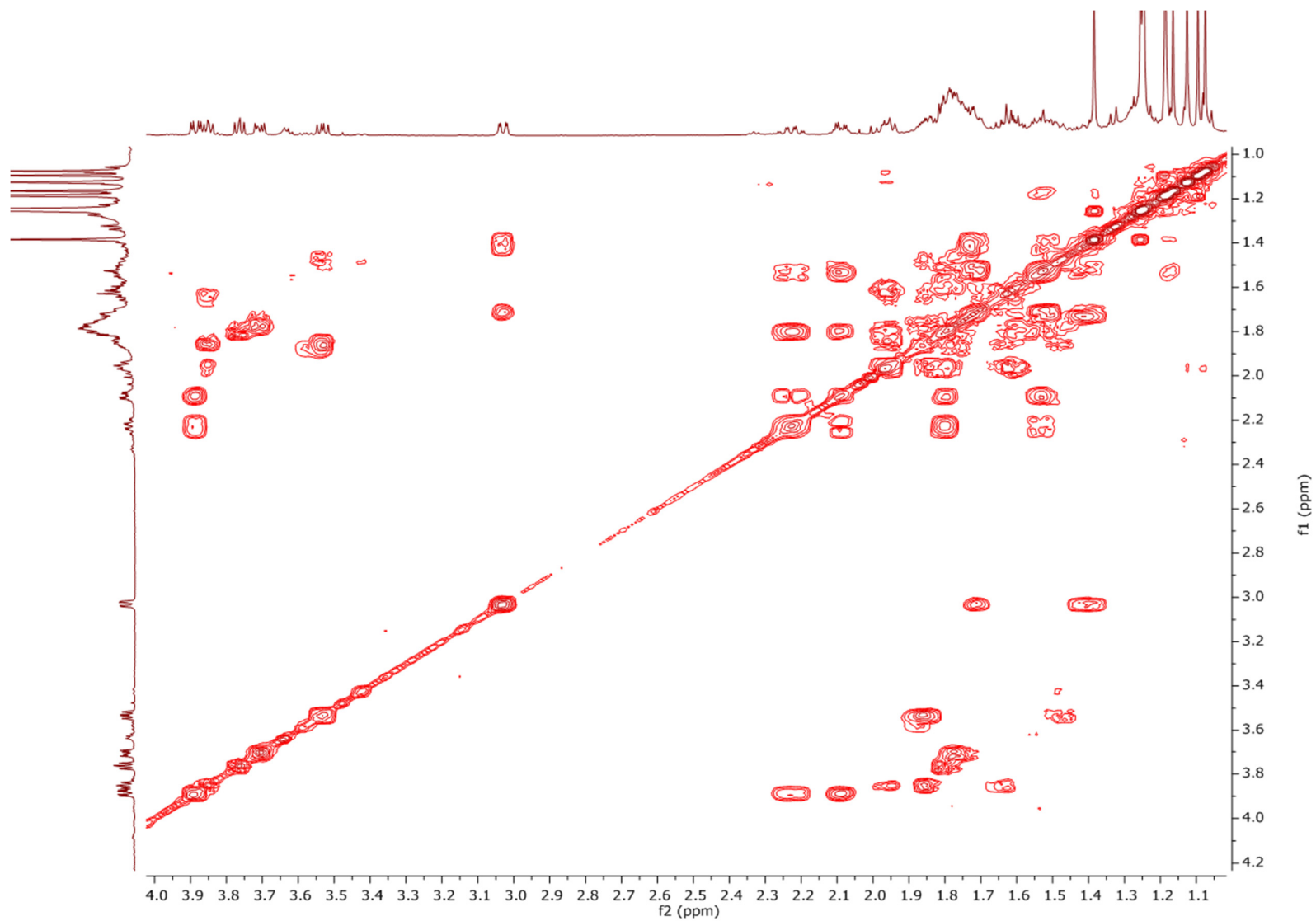


Figure S21. ^1H - ^1H COSY NMR spectrum (600MHz, CDCl_3 , 303K) of compound 4

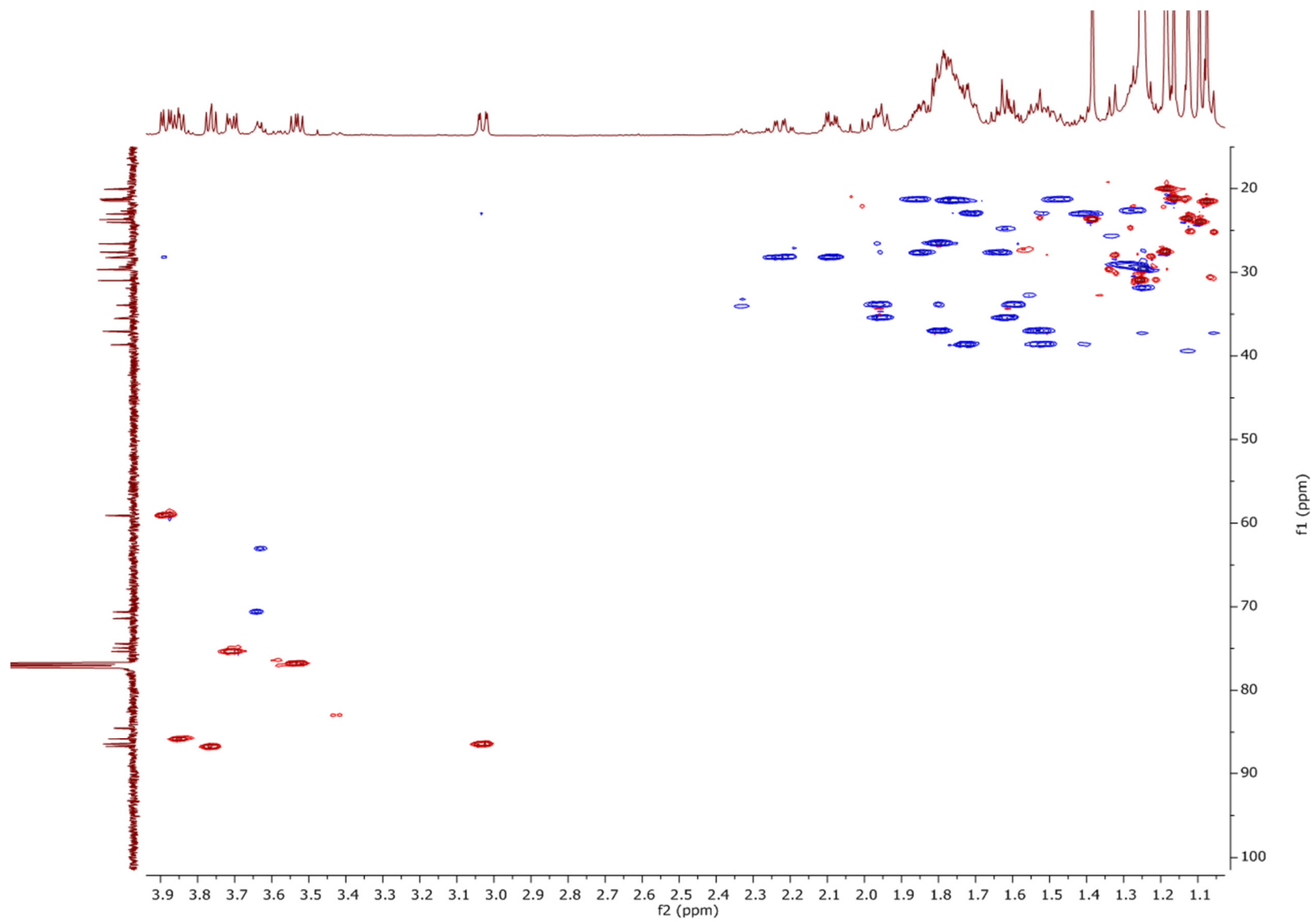


Figure S22. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compound 4

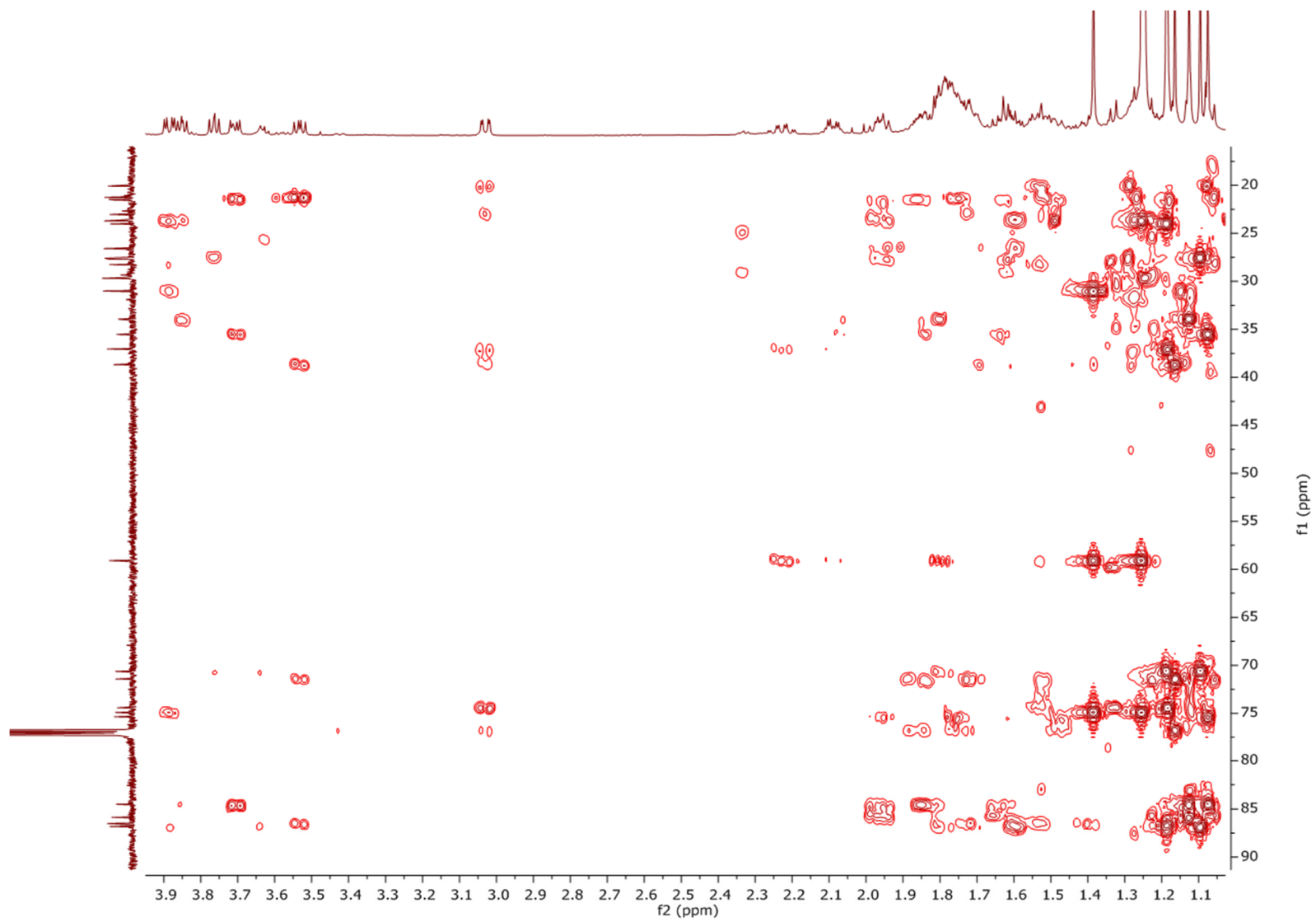


Figure S23. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound 4

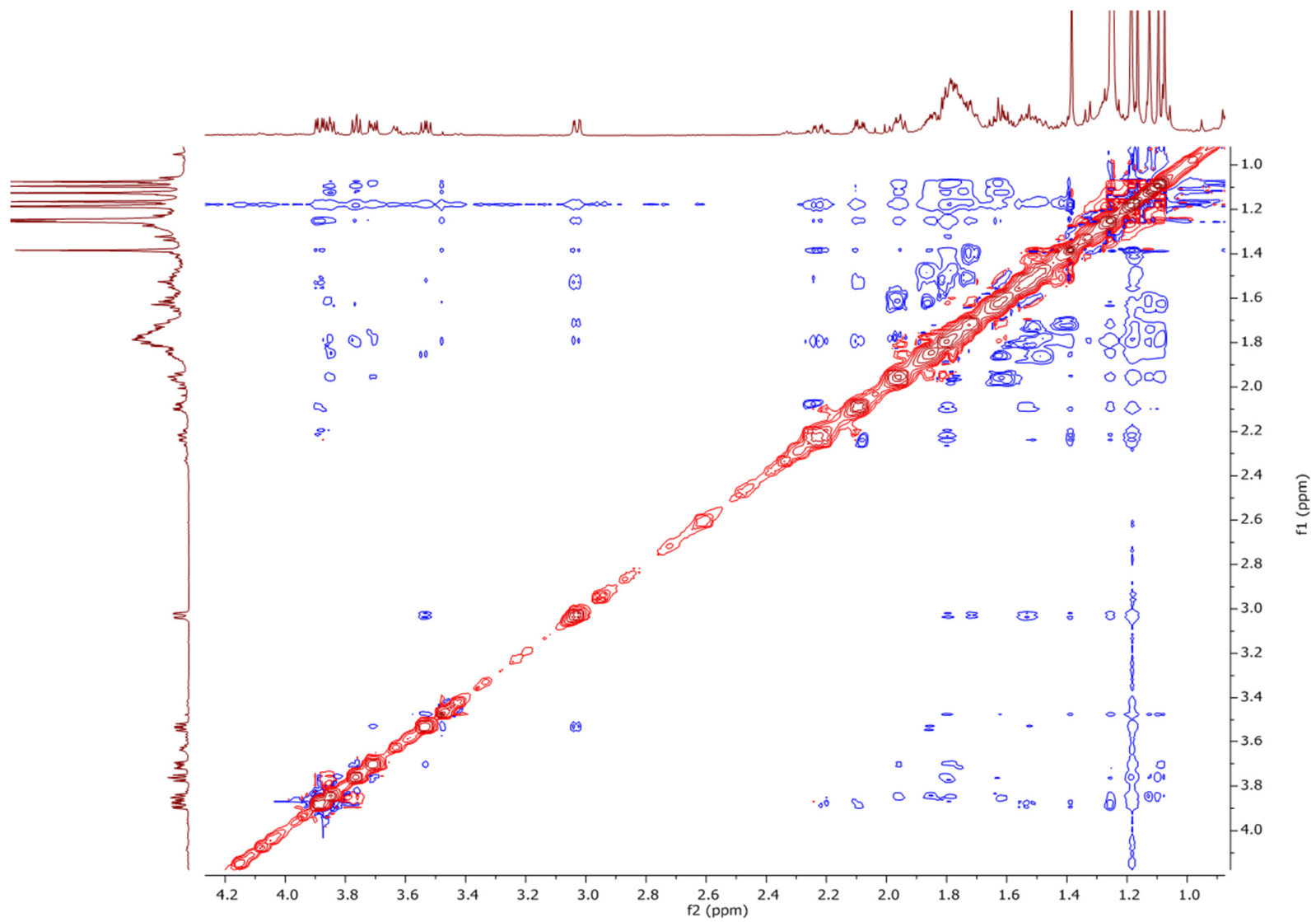


Figure S24. ROESY NMR spectrum (600MHz, CDCl₃, 303K) of compound 4

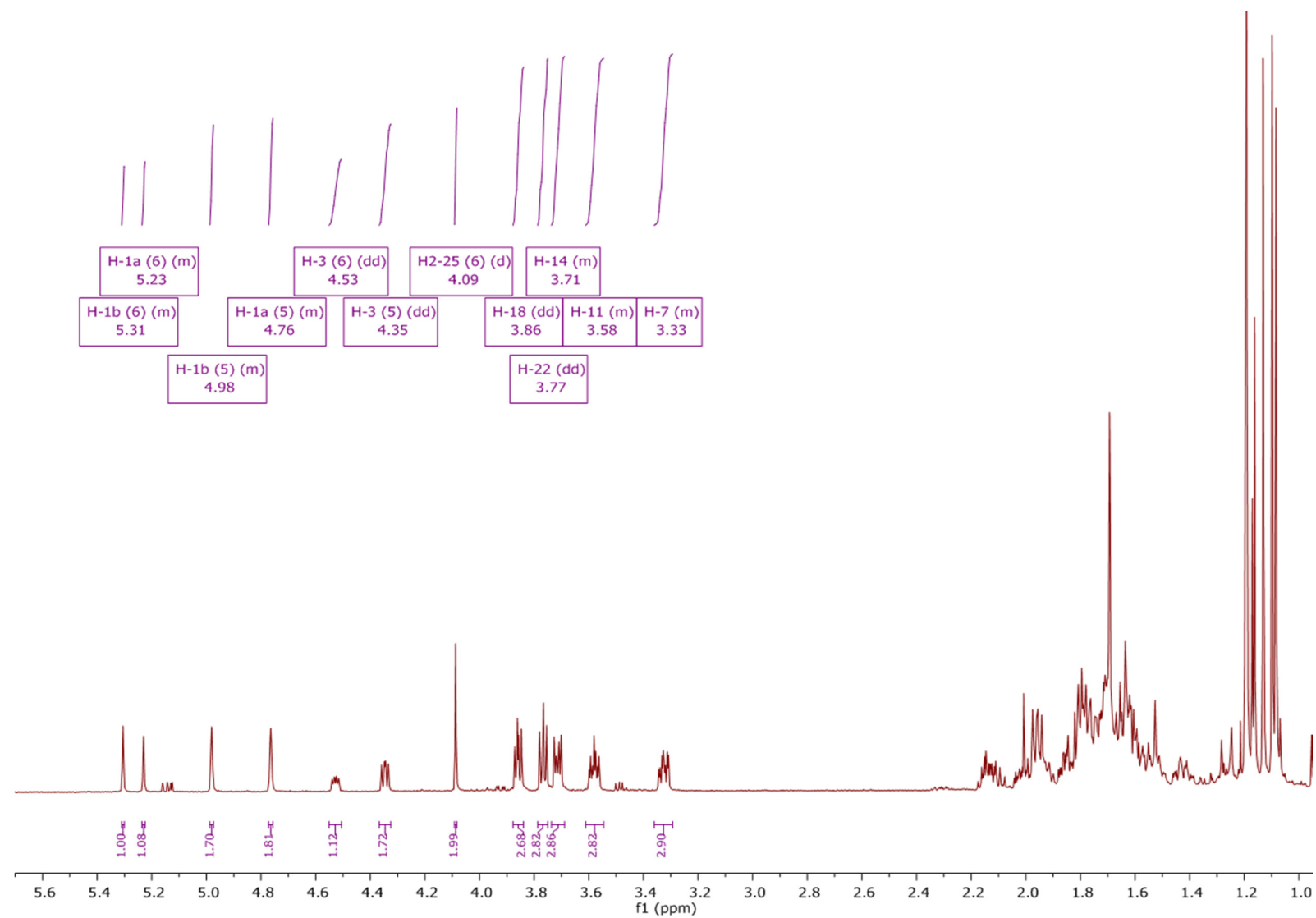


Figure S25. $^1\text{H-NMR}$ spectrum (600MHz, CDCl_3 , 303K) of compounds 5 and 6

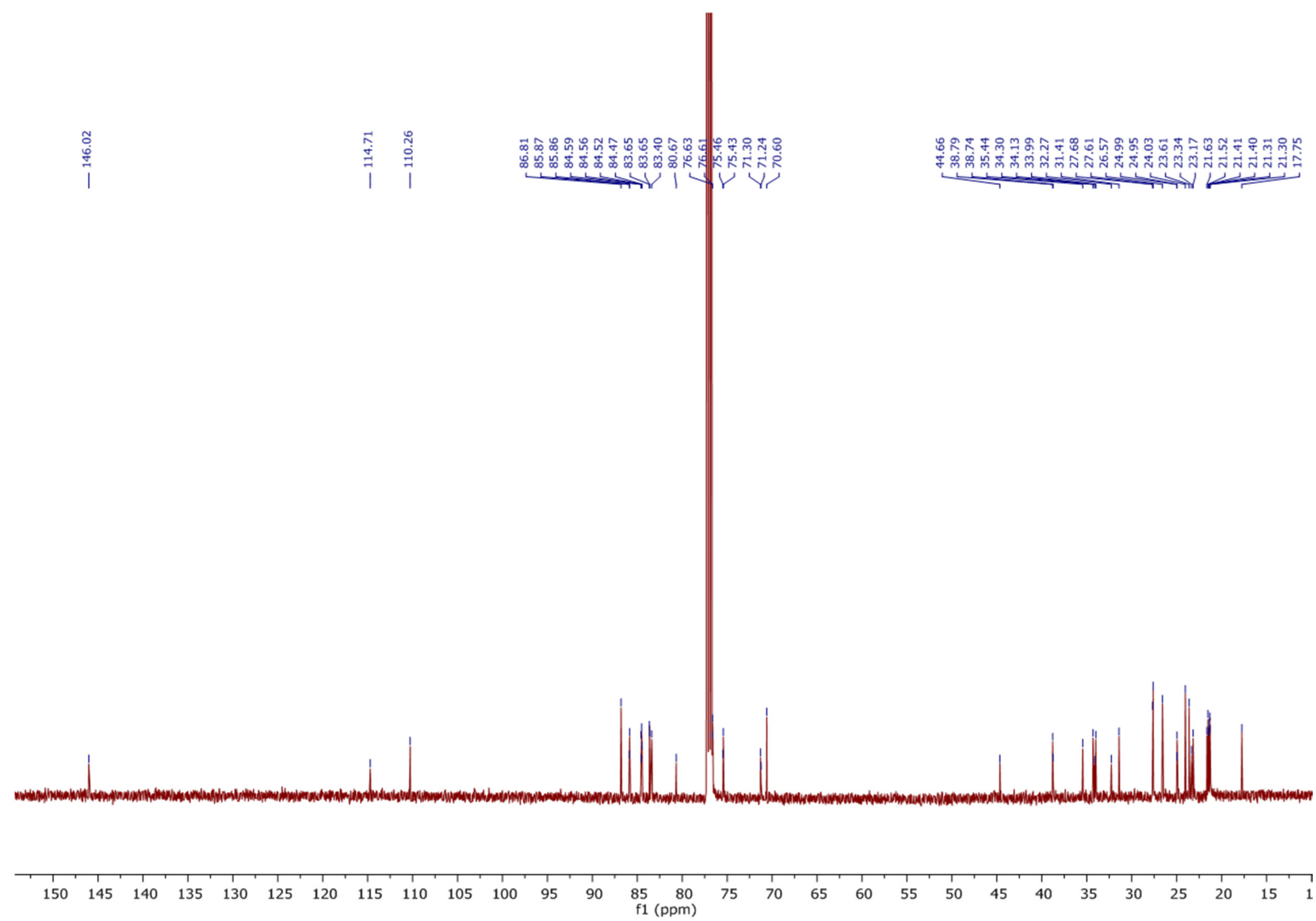


Figure S26. ^{13}C -NMR spectrum (150MHz, CDCl_3 , 303K) of compounds 5 and 6

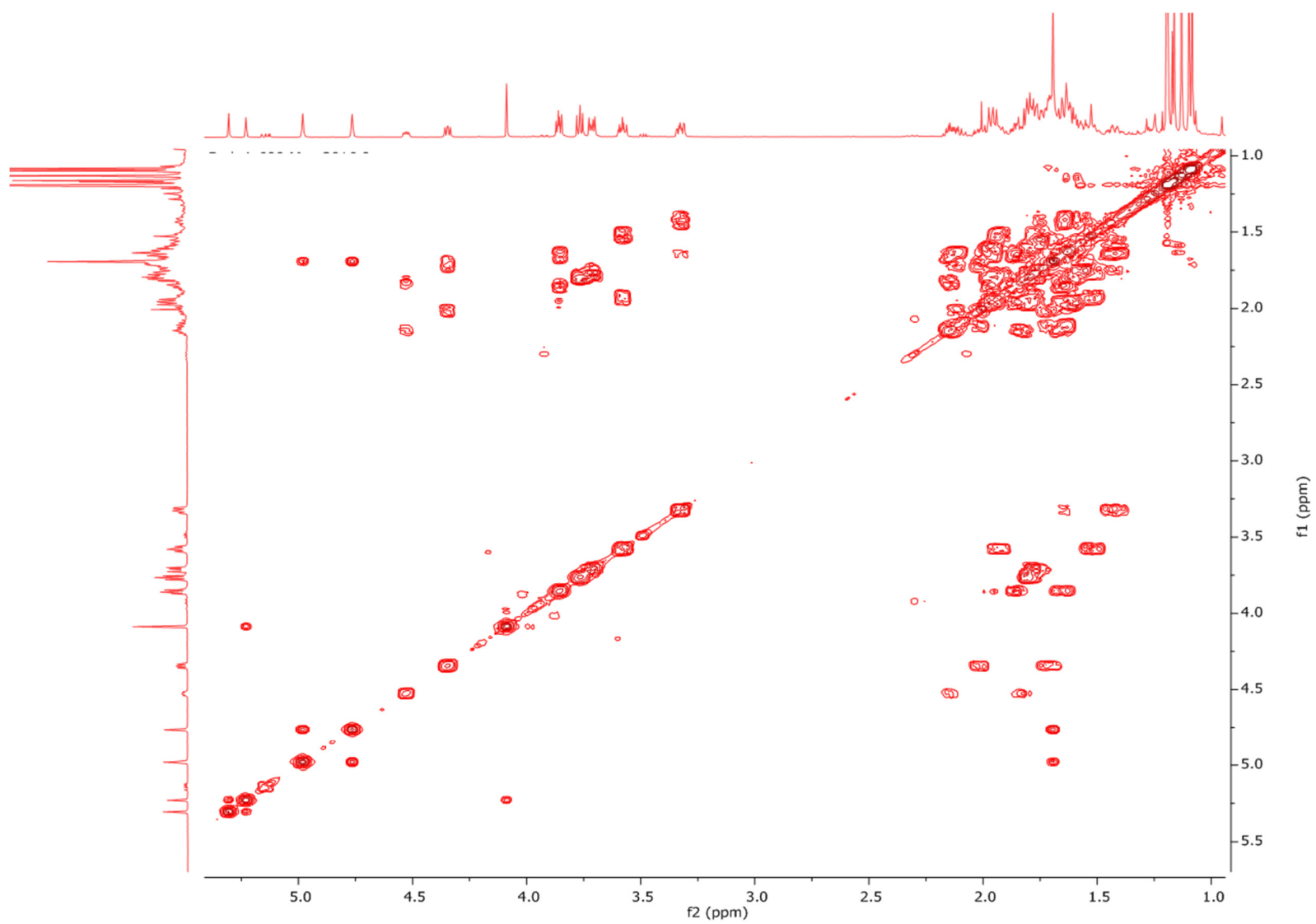


Figure S27. ¹H-¹H COSY NMR spectrum (600MHz, CDCl₃, 303K) of compounds **5** and **6**

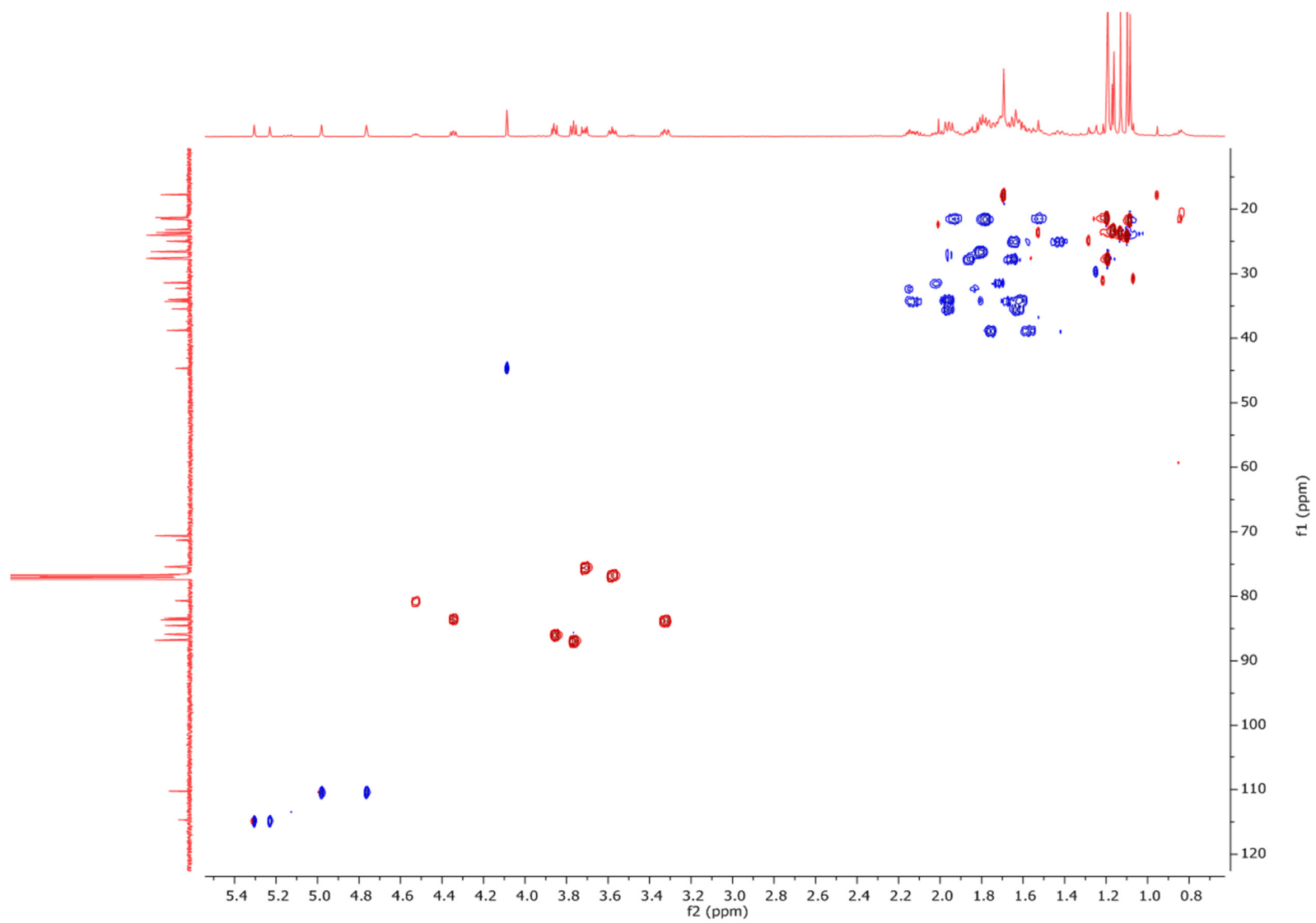


Figure S28. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compounds 5 and 6

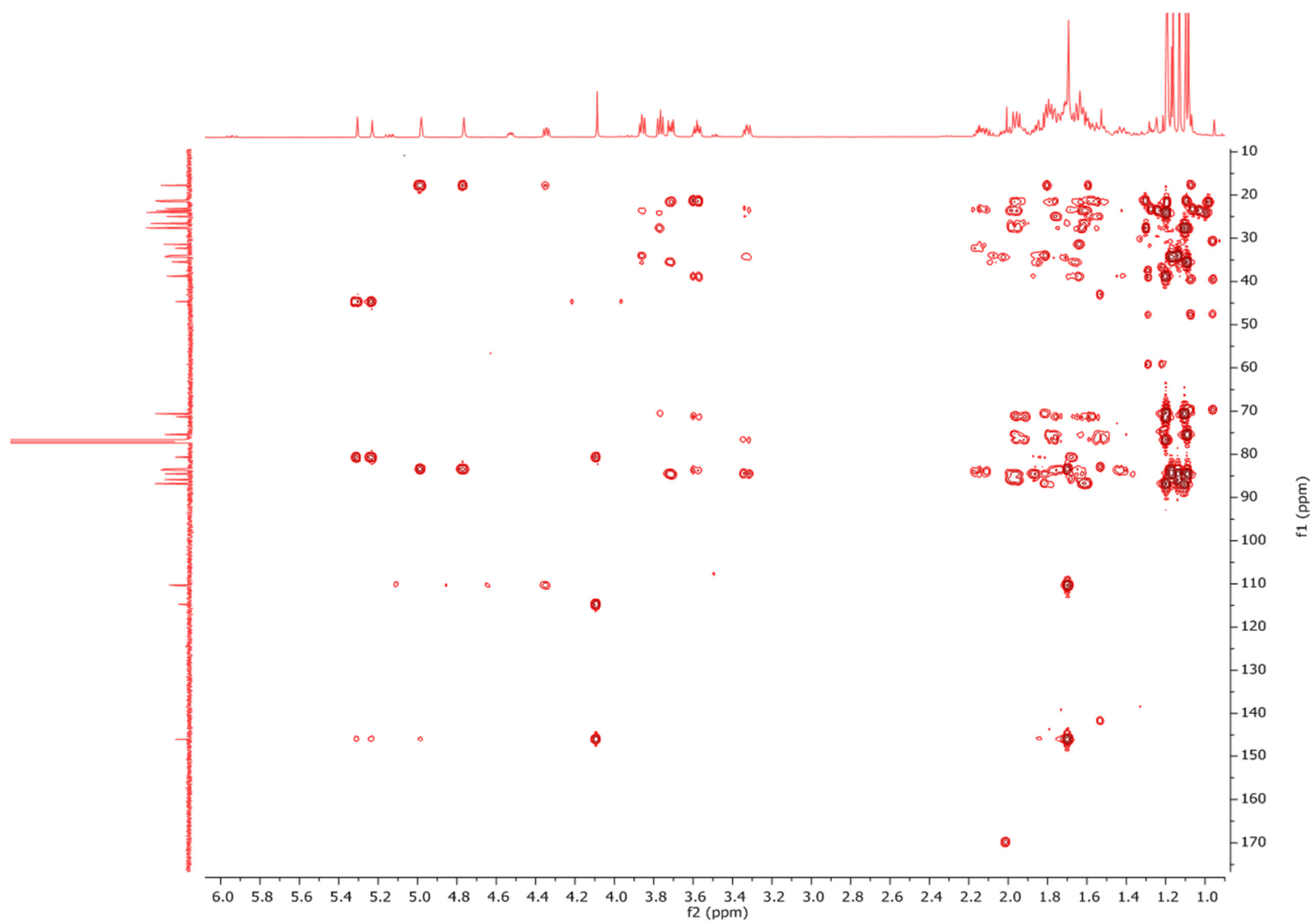


Figure S29. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compounds 5 and 6

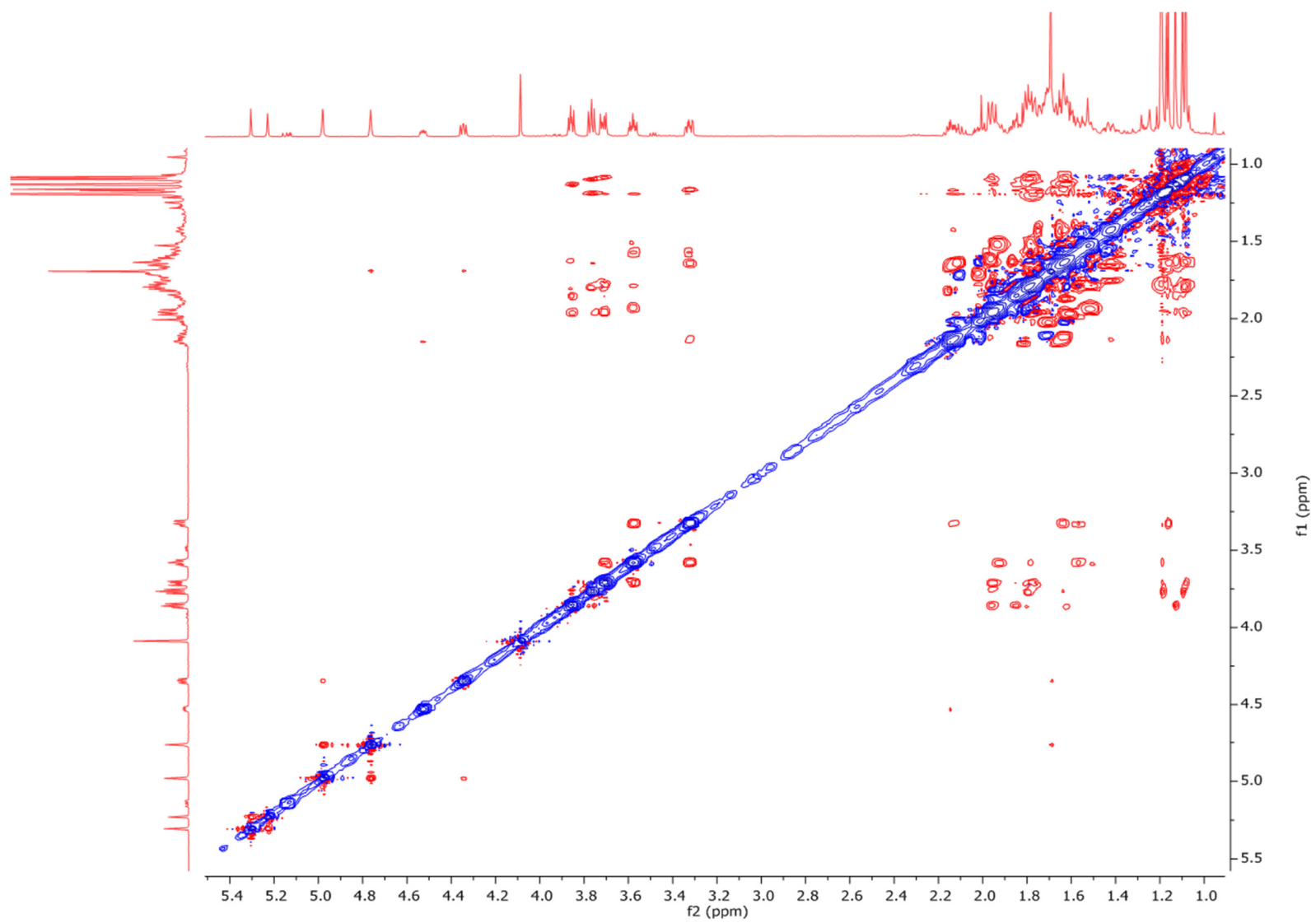


Figure S30. ROESY NMR spectrum (600MHz, CDCl₃, 303K) of compounds **5** and **6**

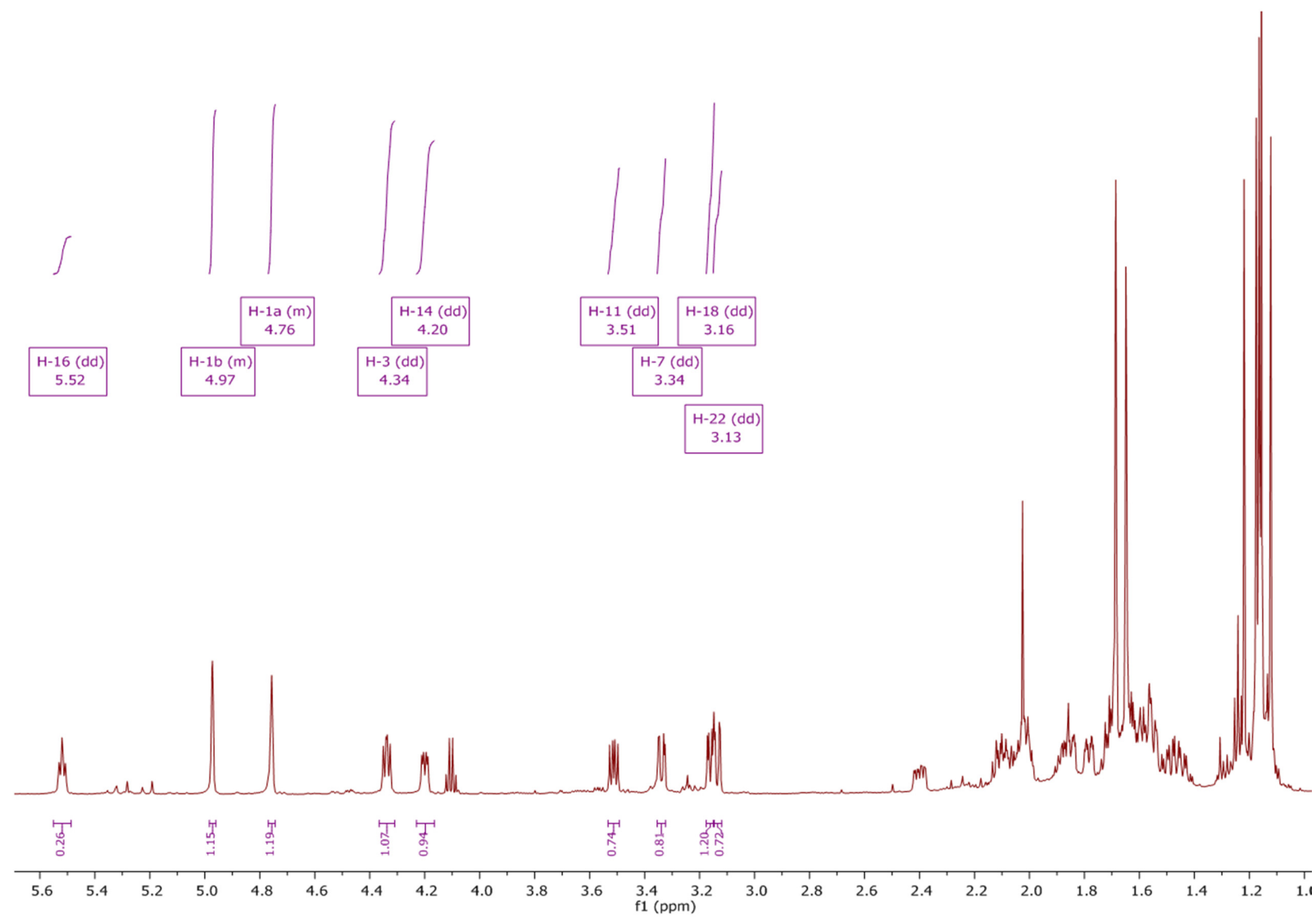


Figure S31. ¹H-NMR spectrum (600MHz, CDCl₃, 303K) of compound 7

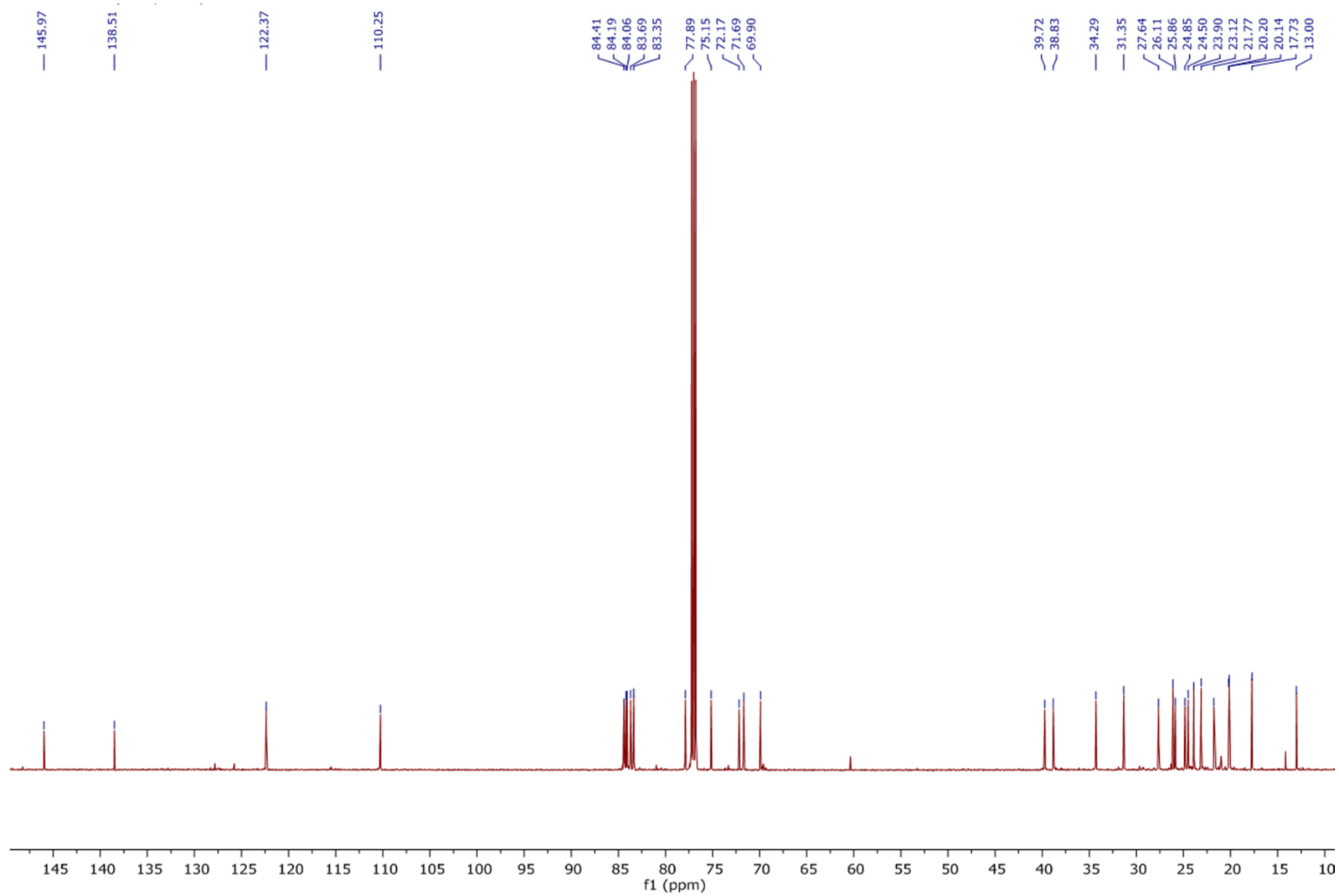


Figure S32. ^{13}C -NMR spectrum (150MHz, CDCl_3 , 303K) of compound 7

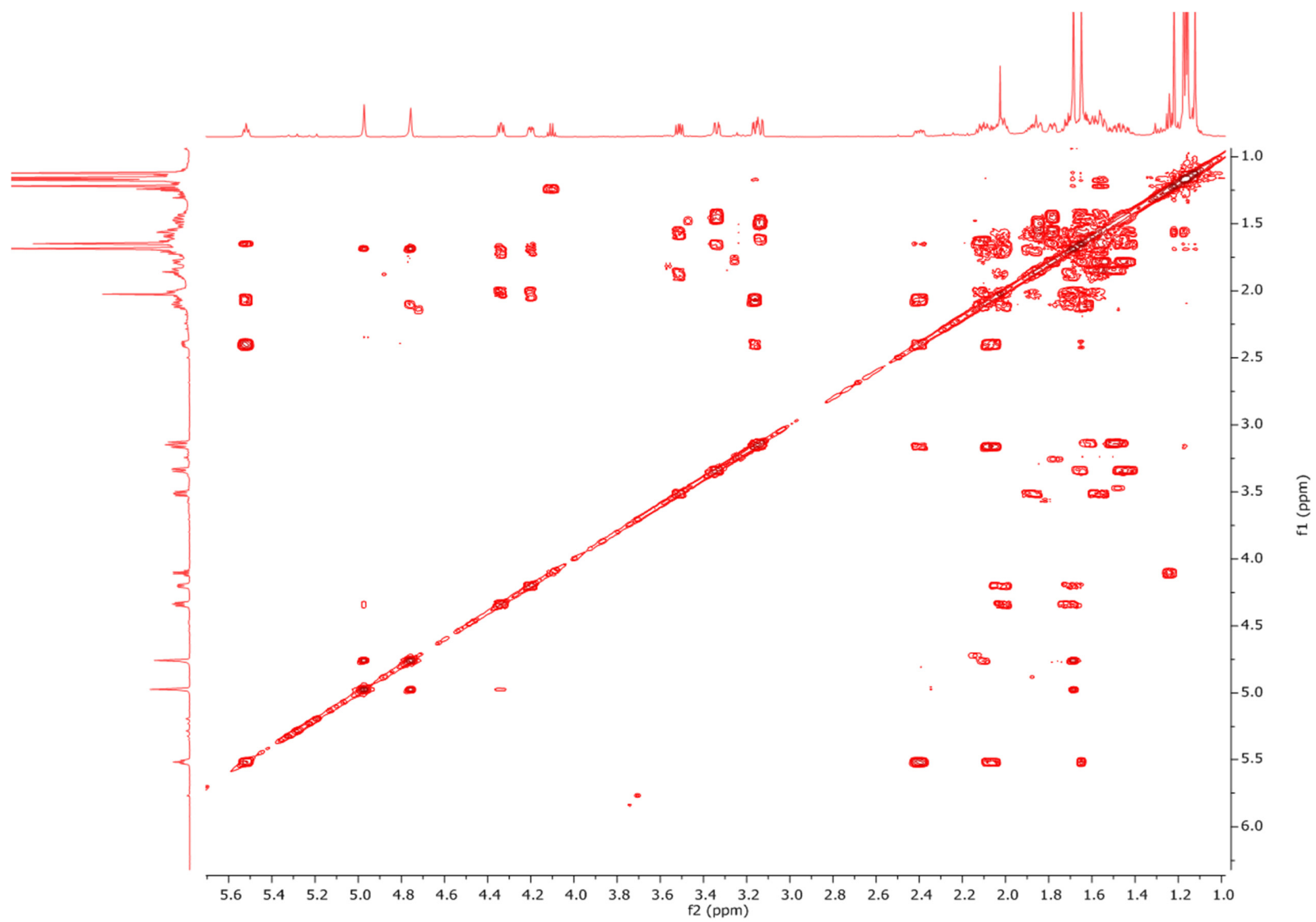


Figure S33. ^1H - ^1H COSY NMR spectrum (600MHz, CDCl_3 , 303K) of compound 7

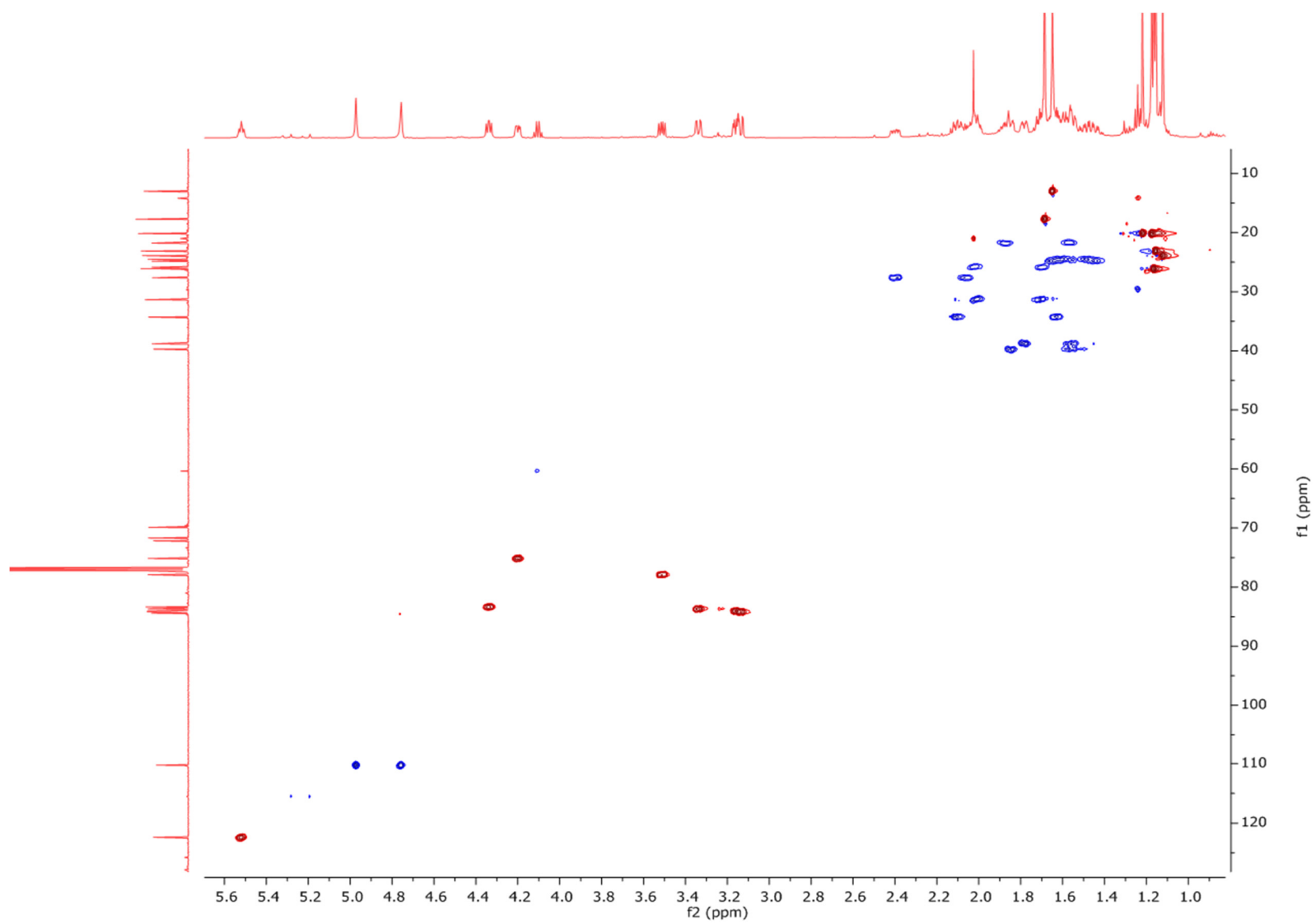


Figure S34. HSQC-DEPT NMR spectrum (600MHz, CDCl_3 , 303K) of compound 7

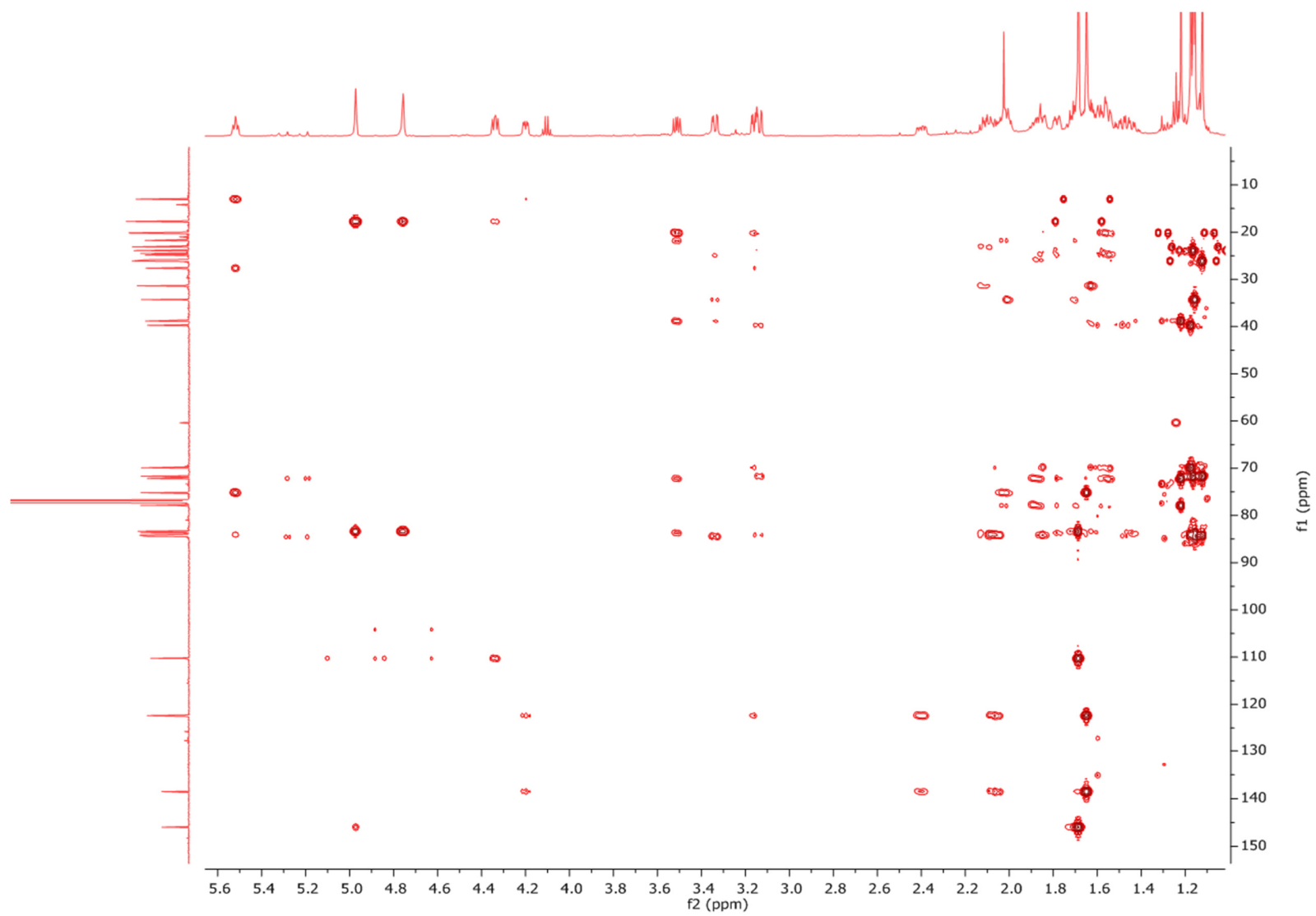


Figure S35. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound 7

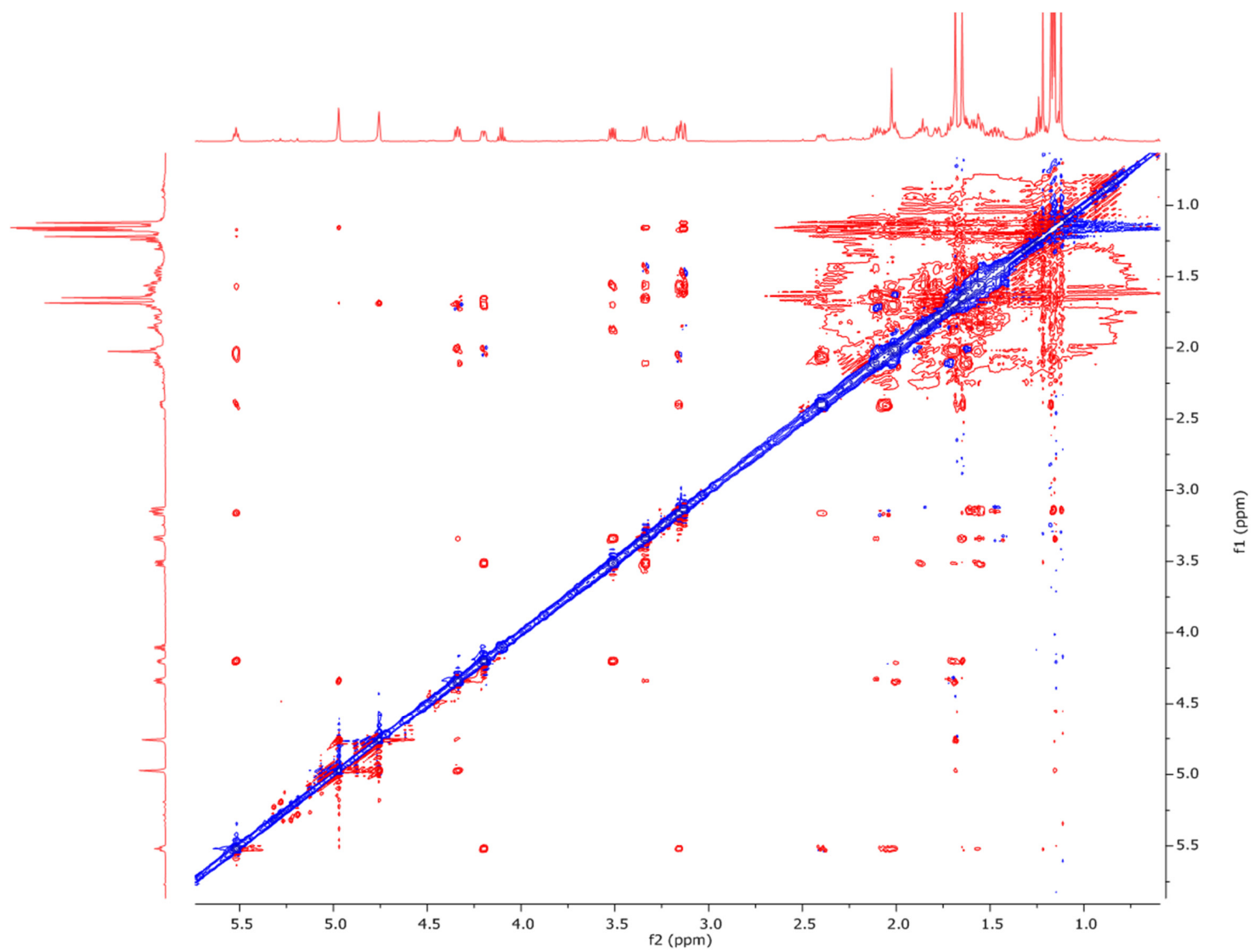


Figure S36. ROESY NMR spectrum (600MHz, CDCl₃, 303K) of compound **7**

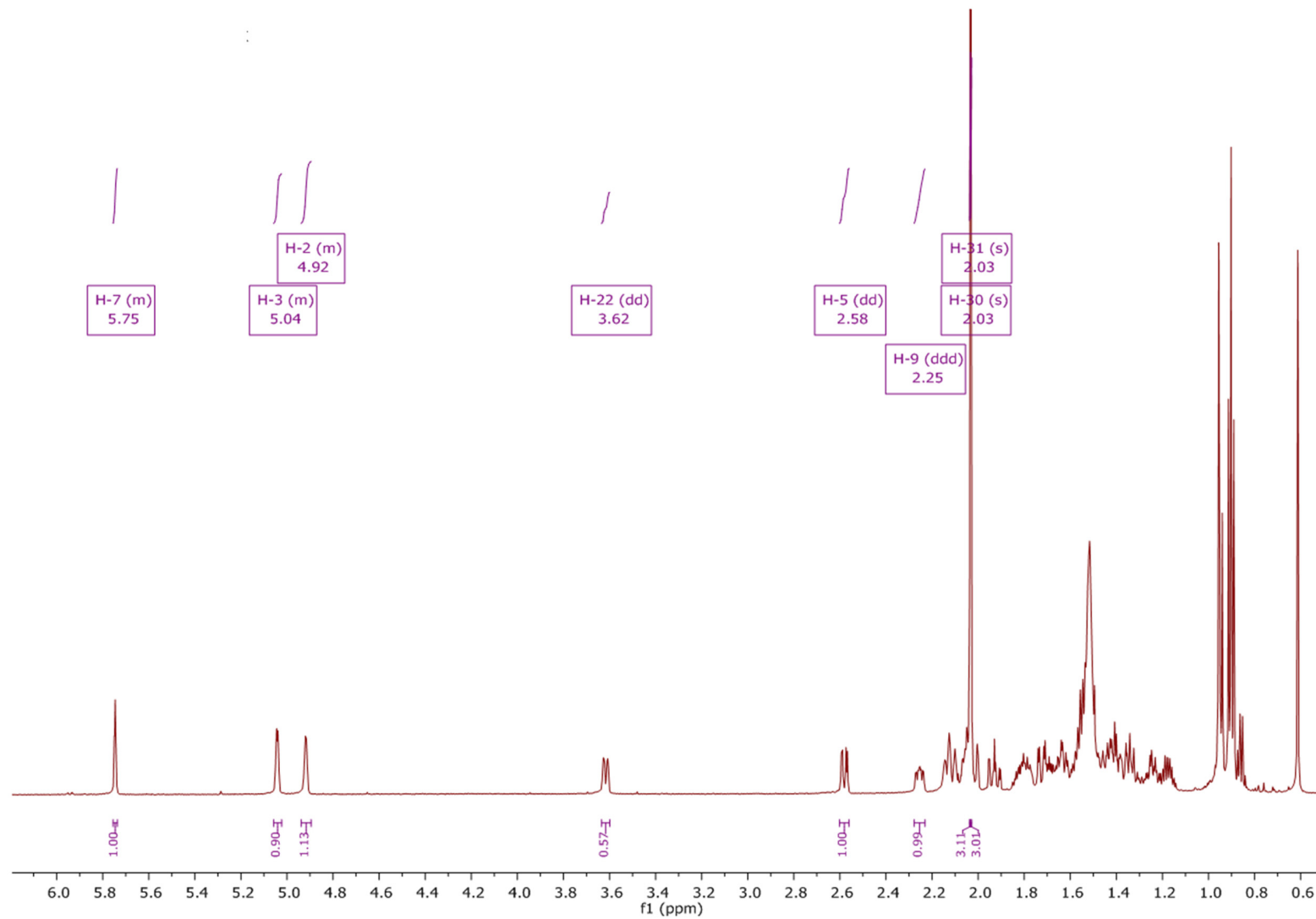


Figure S37. ¹H-NMR spectrum (600MHz, CDCl₃, 303K) of compound 8

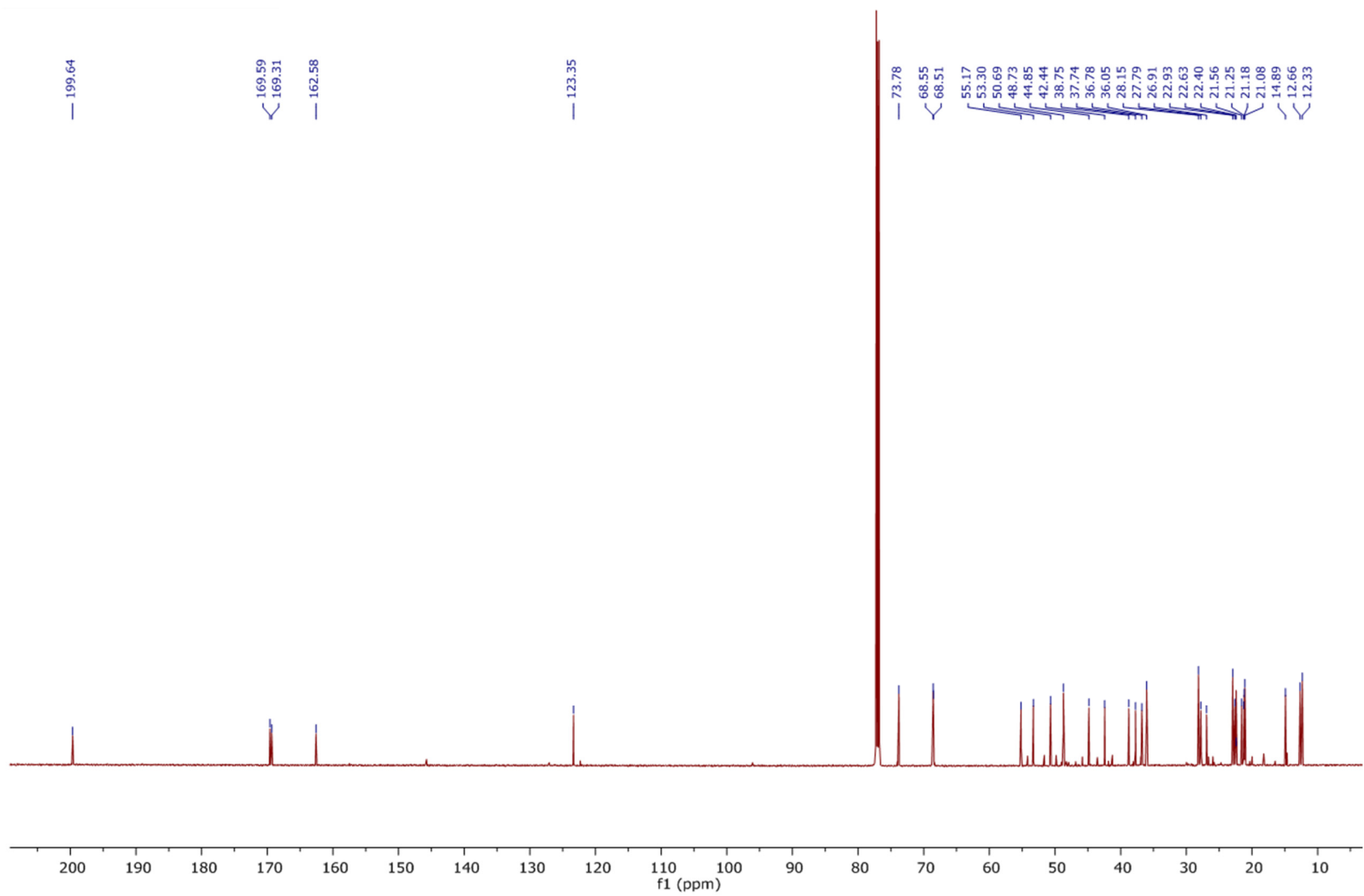


Figure S38. ^{13}C -NMR spectrum (150MHz, CDCl_3 , 303K) of compound 8

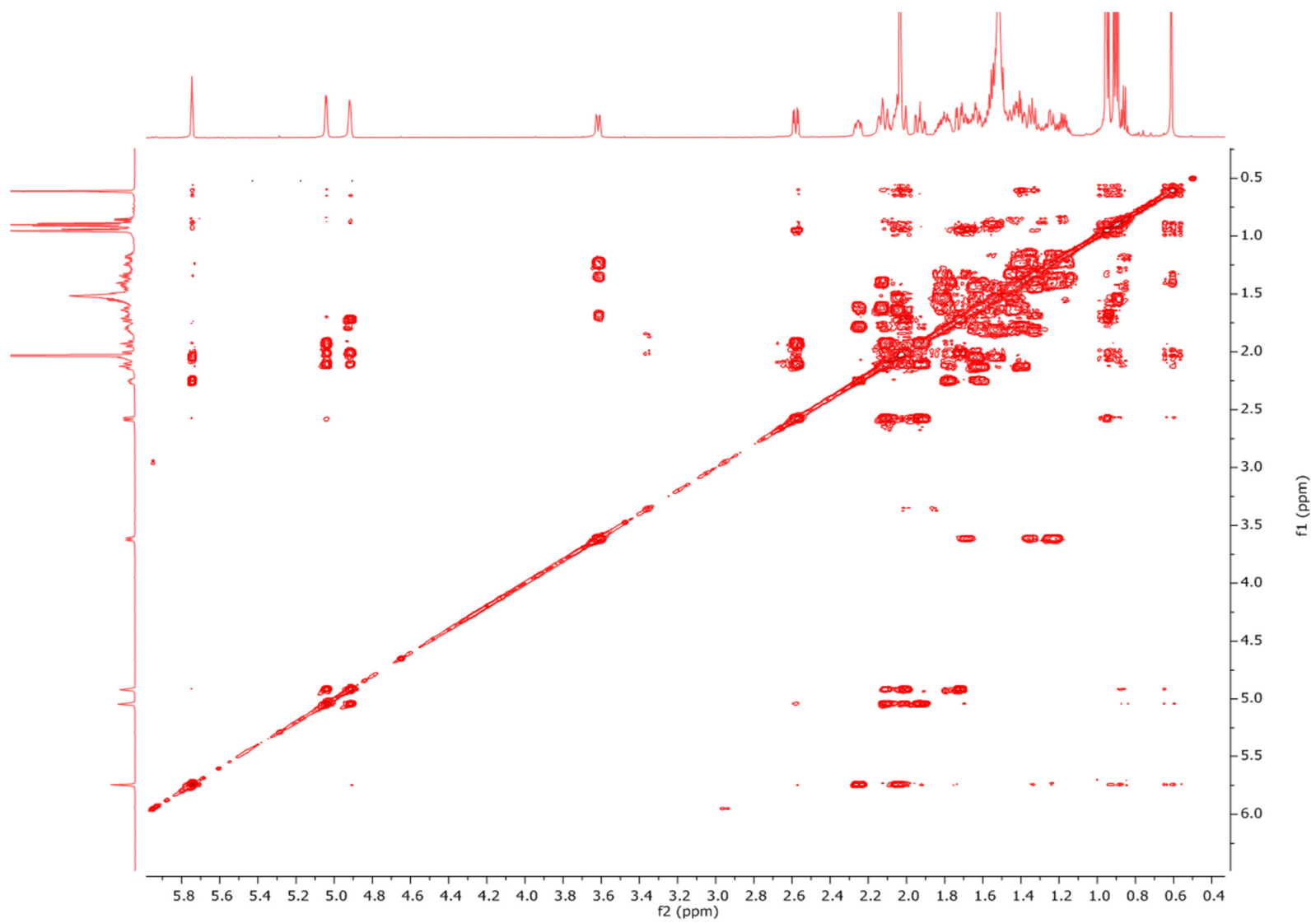


Figure S39. ^1H - ^1H COSY NMR spectrum (600MHz, CDCl_3 , 303K) of compound 8

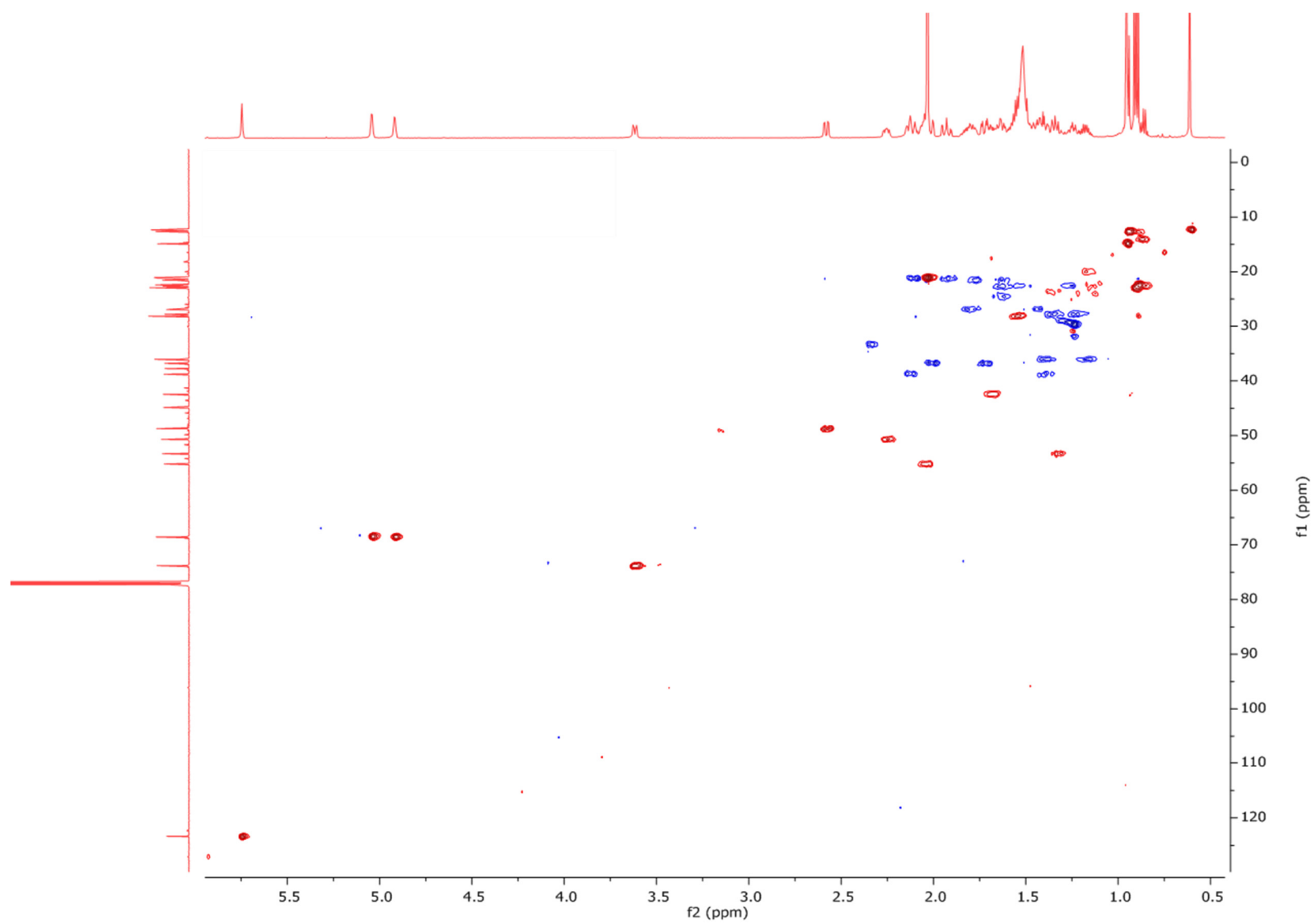


Figure S40. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compound **8**

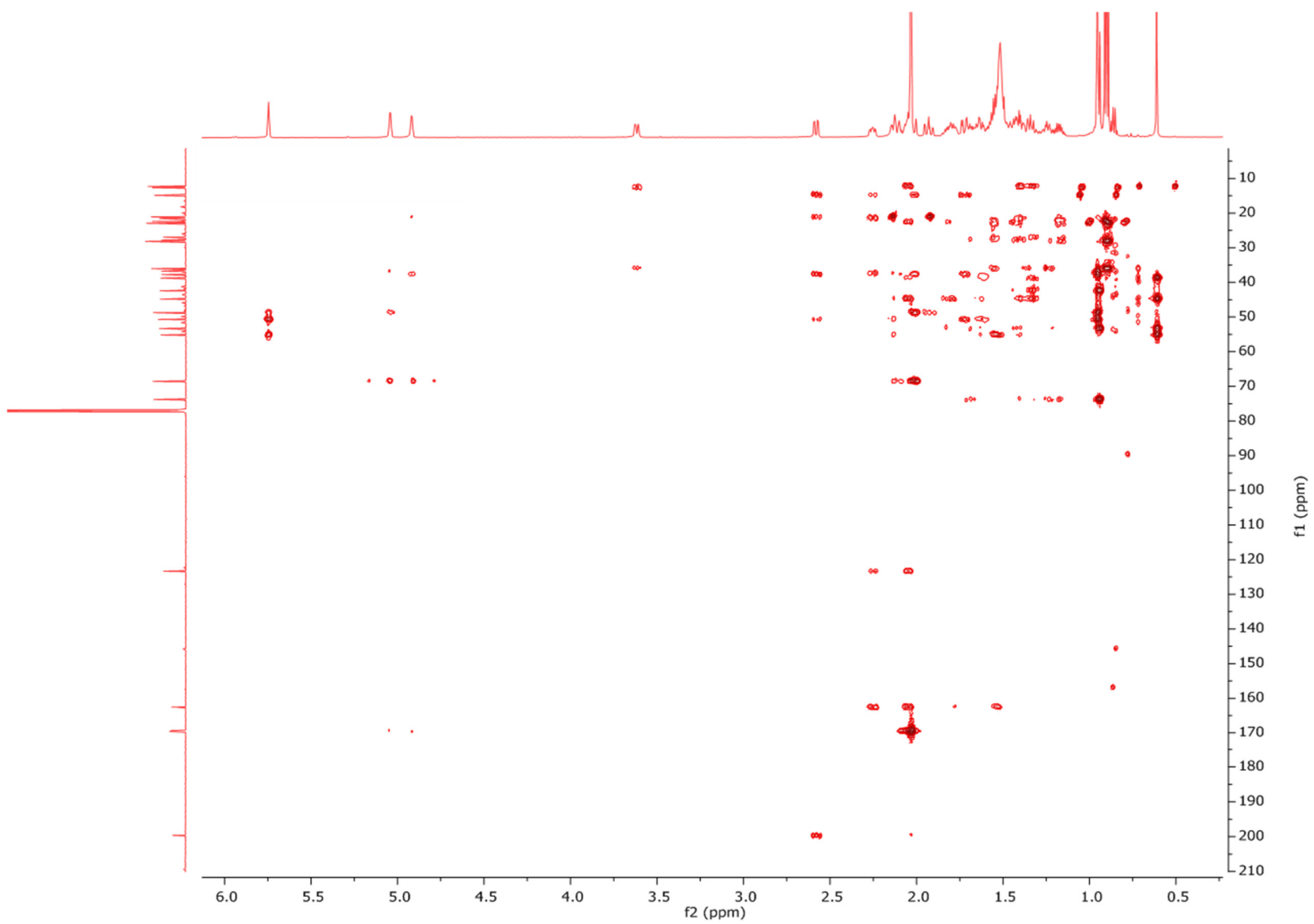


Figure S41. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound **8**

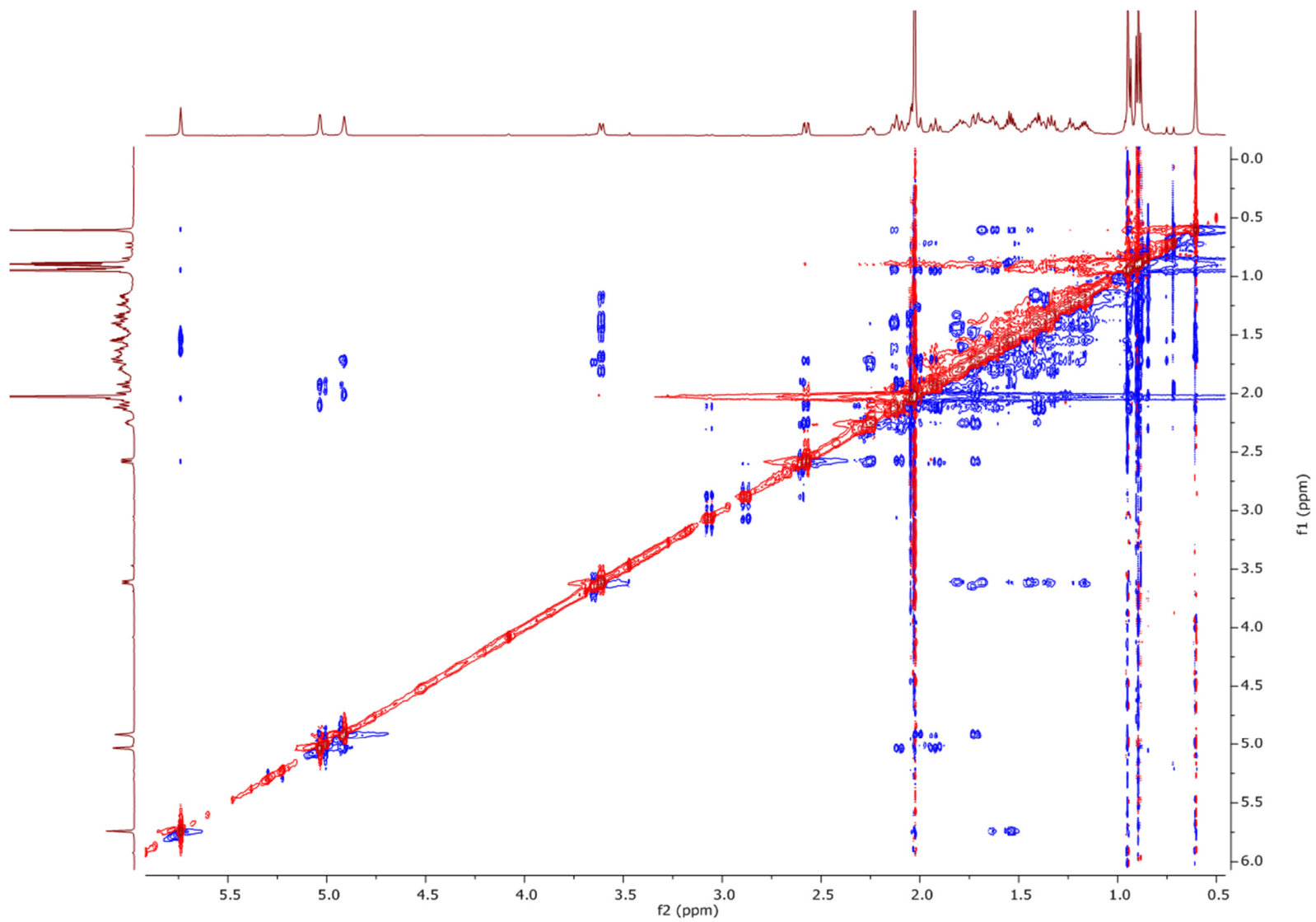


Figure S42. NOESY NMR spectrum (600MHz, CDCl₃, 303K) of compound **8**

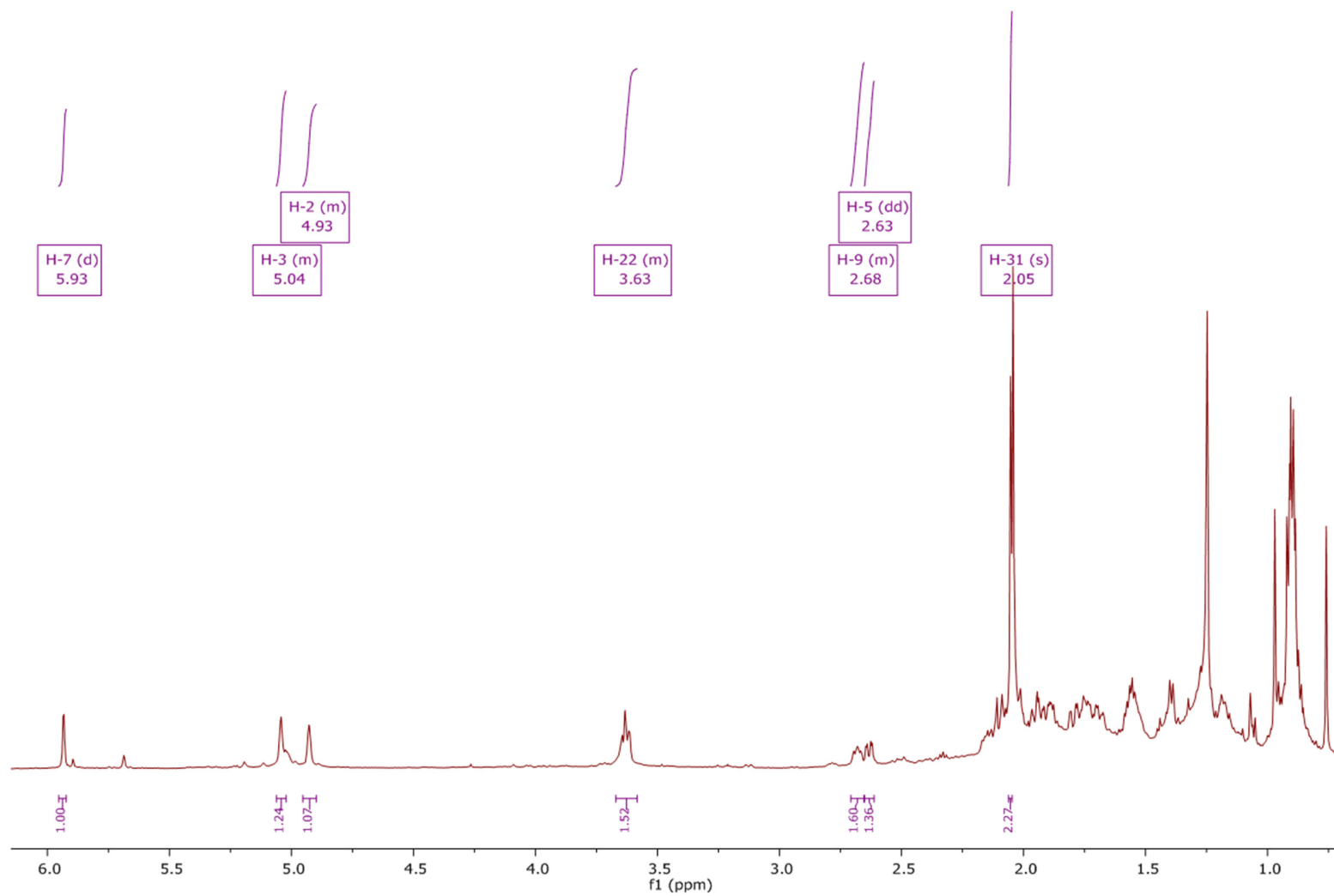


Figure S43. ¹H-NMR spectrum (600MHz, CDCl₃, 303K) of compound 9

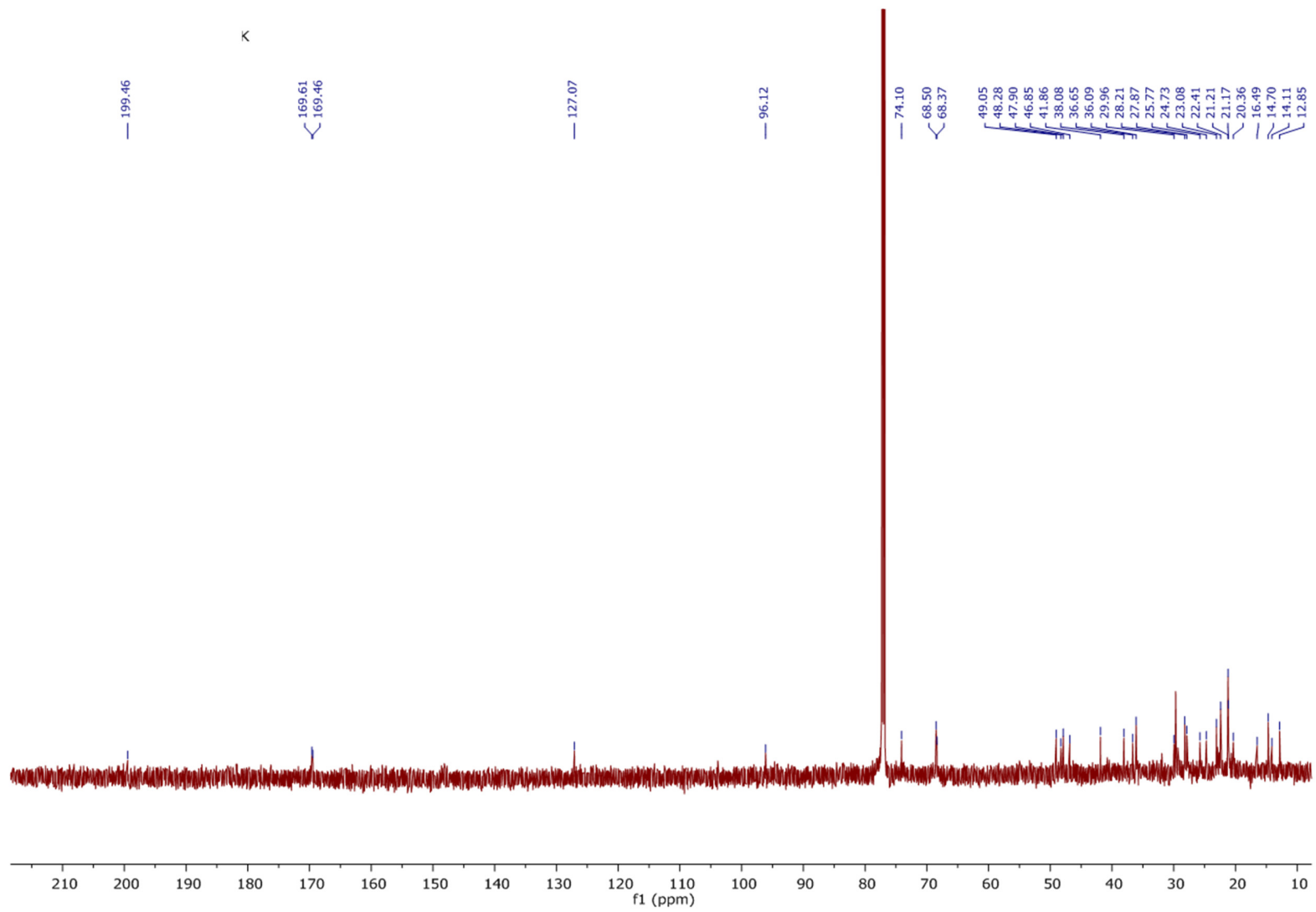


Figure S44. ¹³C-NMR spectrum (150MHz, CDCl₃, 303K) of compound 9

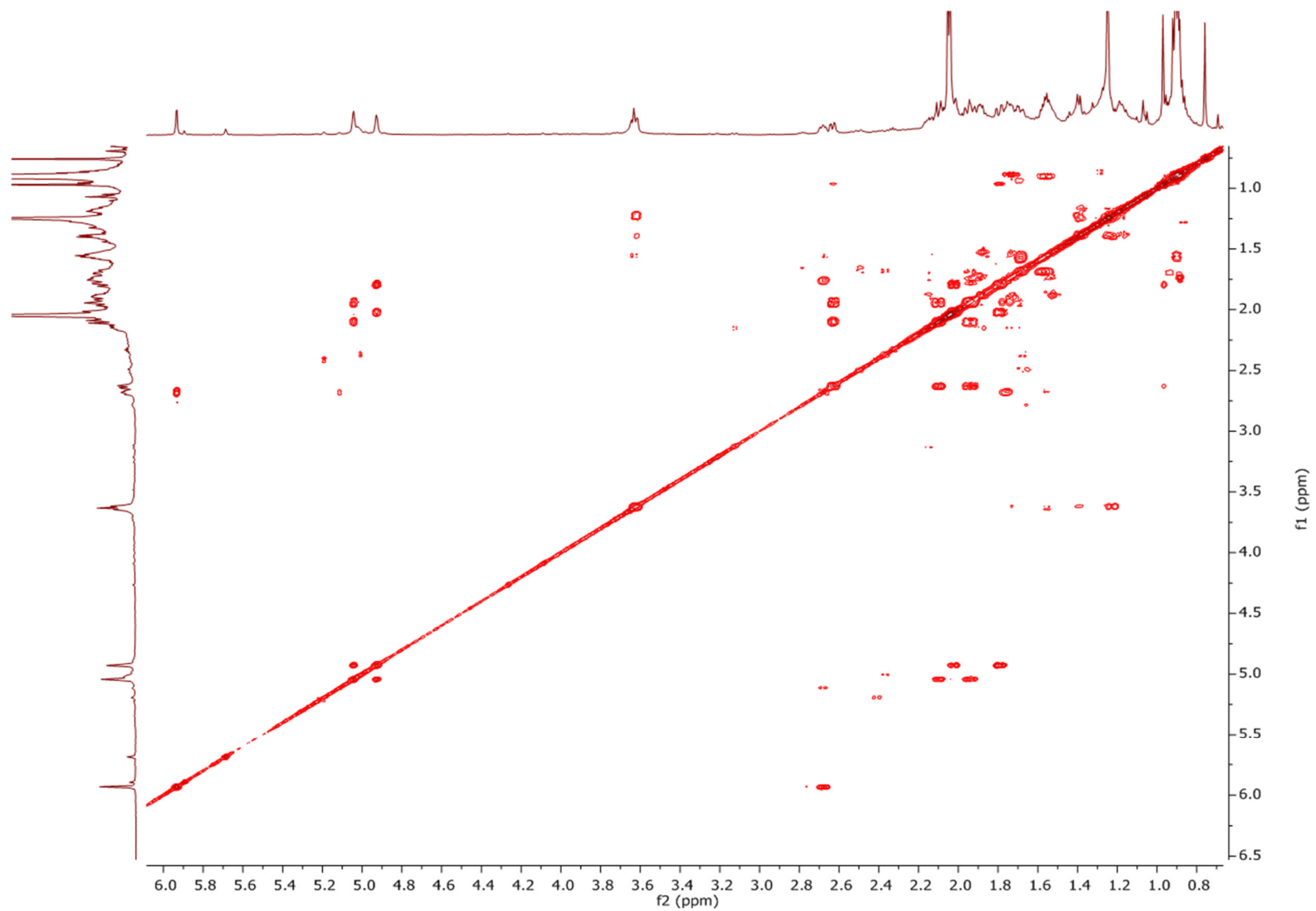


Figure S45. ^1H - ^1H COSY NMR spectrum (600MHz, CDCl_3 , 303K) of compound **9**

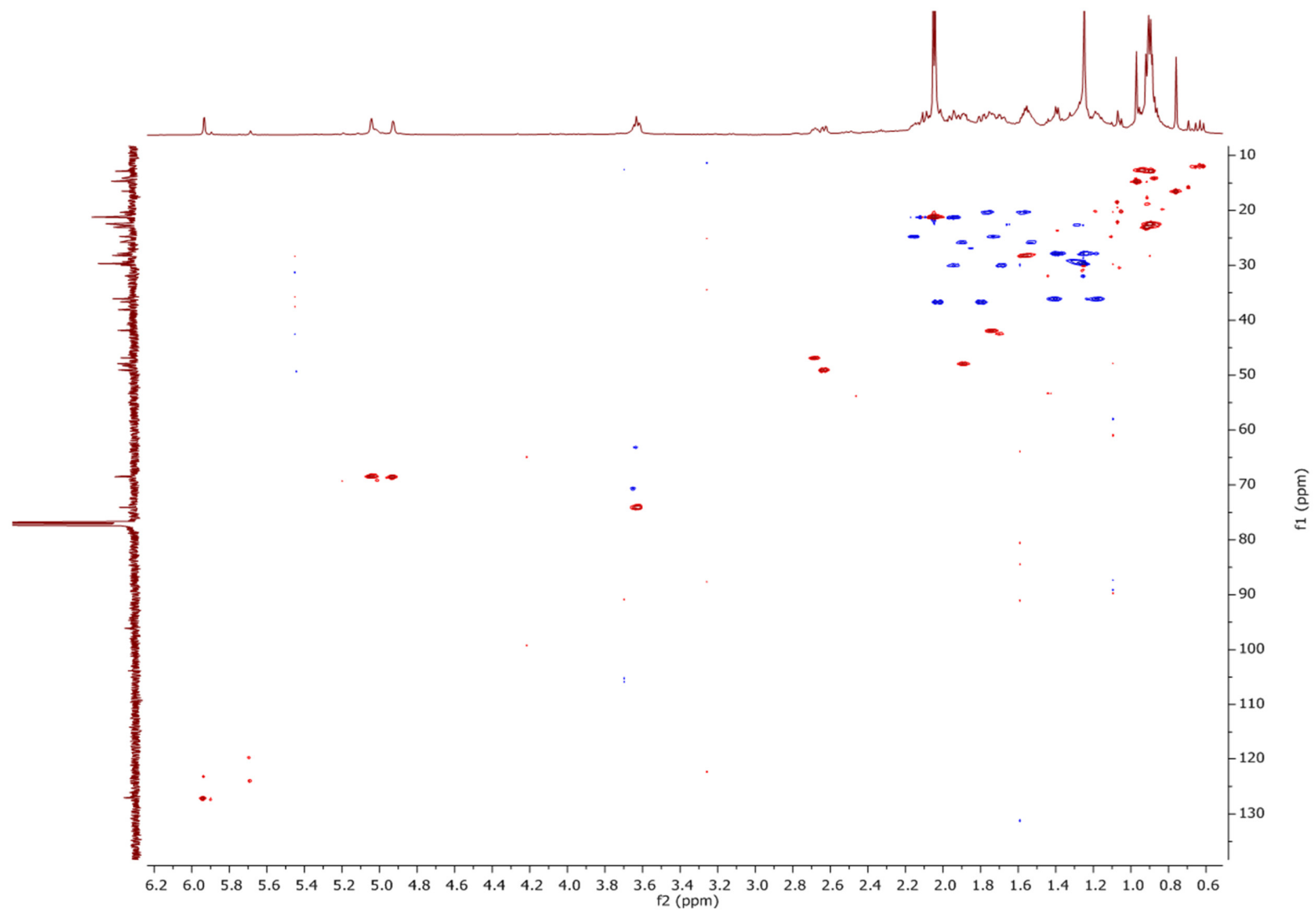


Figure S46. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compound 9

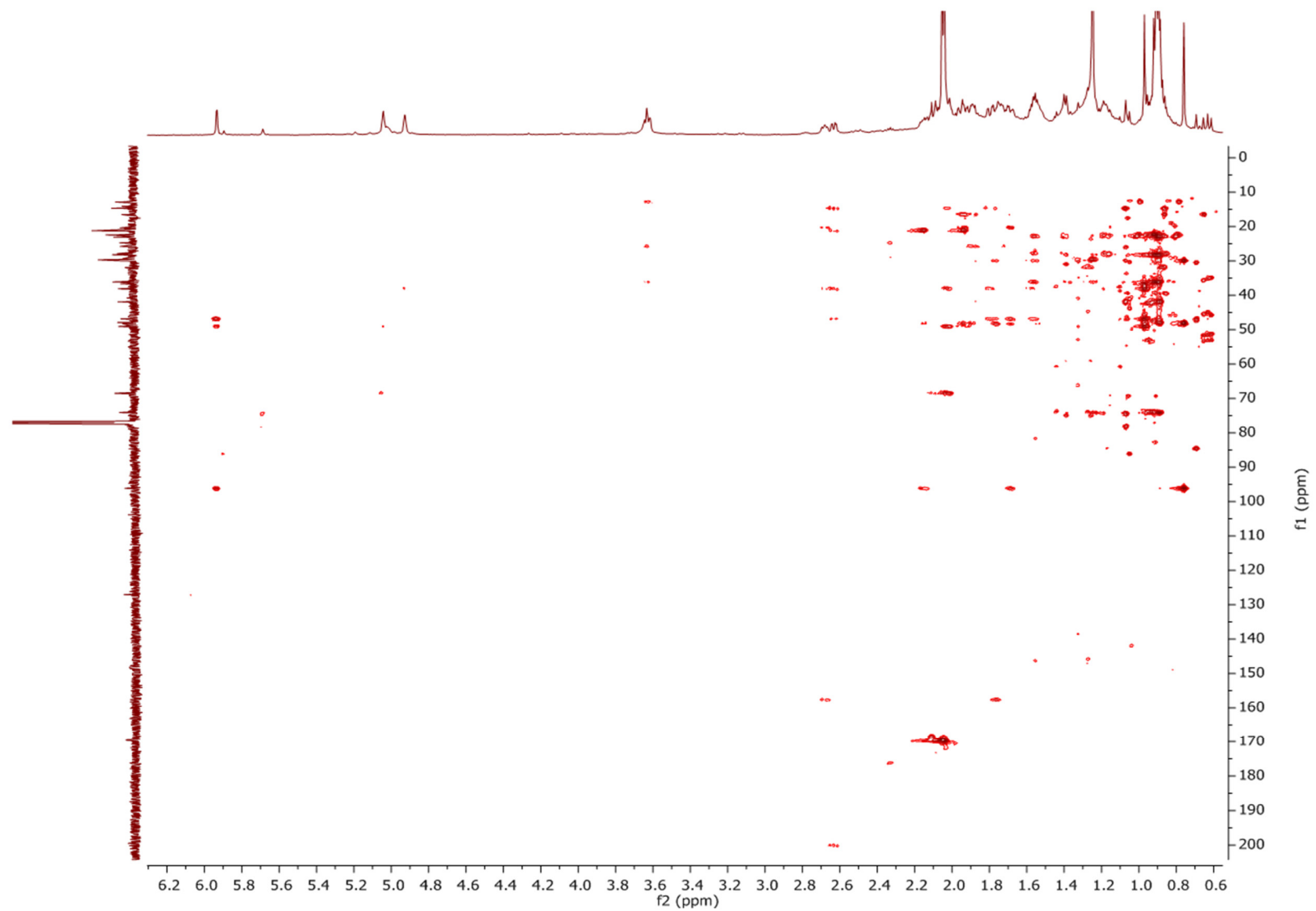


Figure S47. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound 9

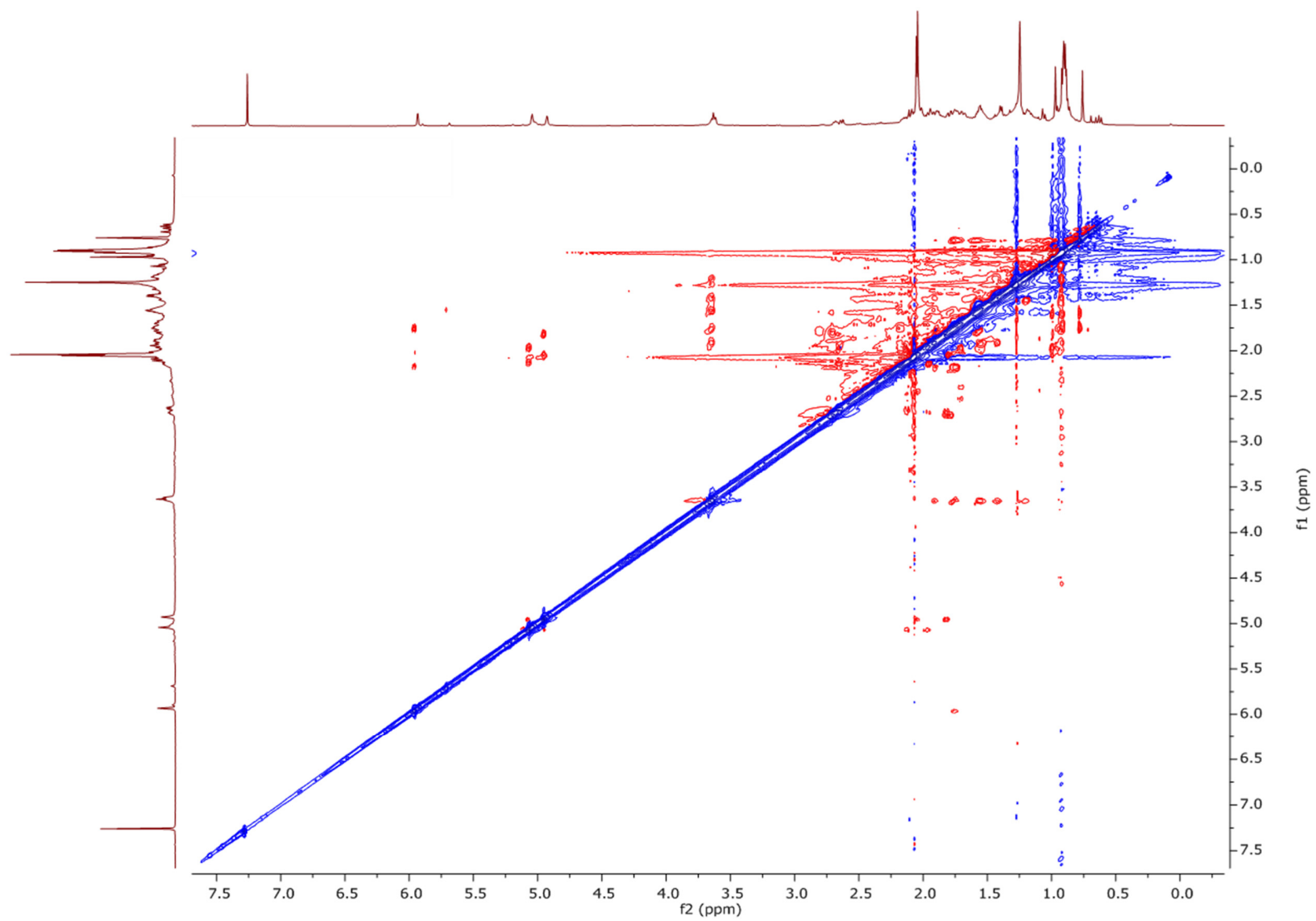


Figure S48. ROESY NMR spectrum (600MHz, CDCl₃, 303K) of compound **9**

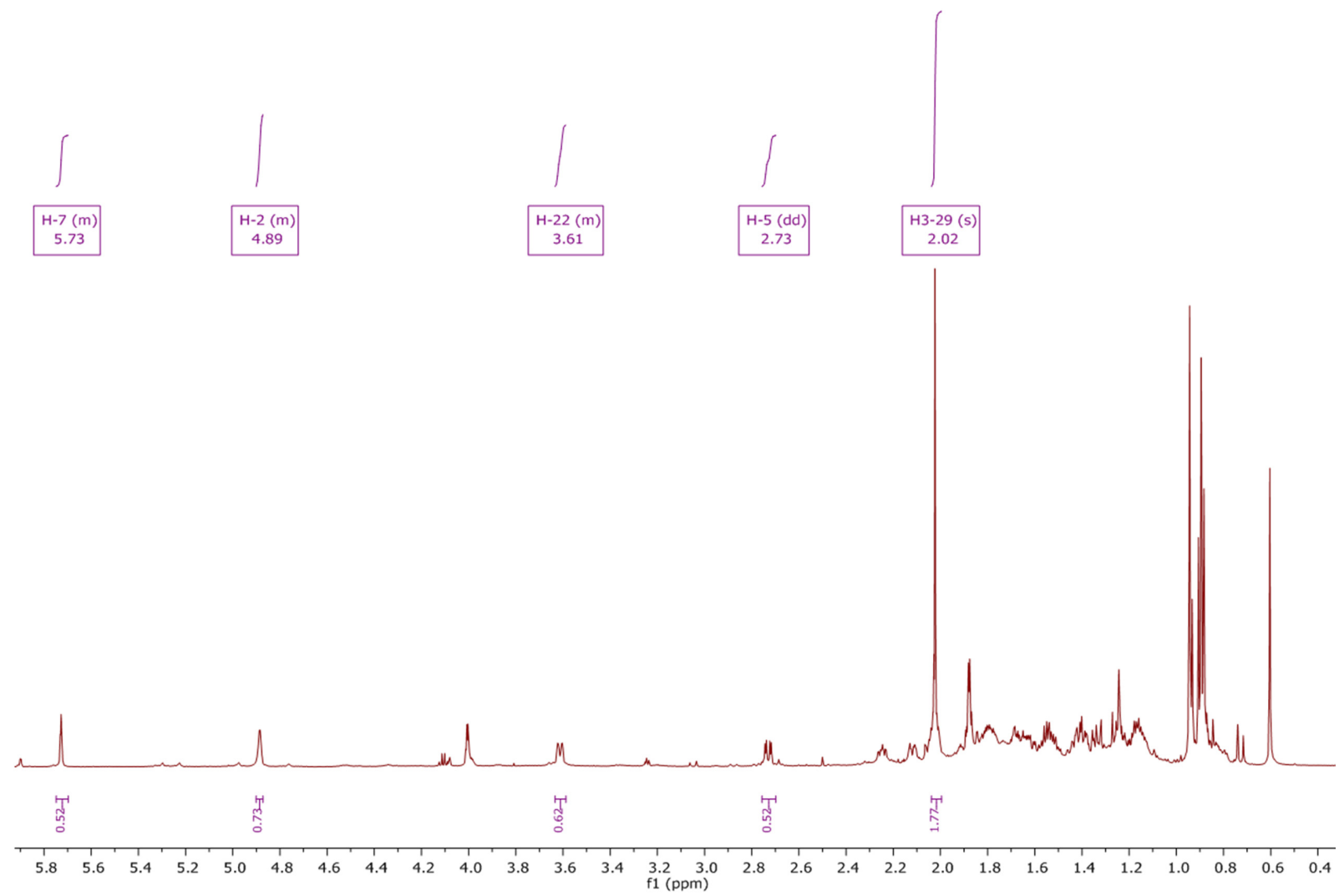


Figure S49. ¹H-NMR spectrum (600MHz, CDCl₃, 303K) of compound 10

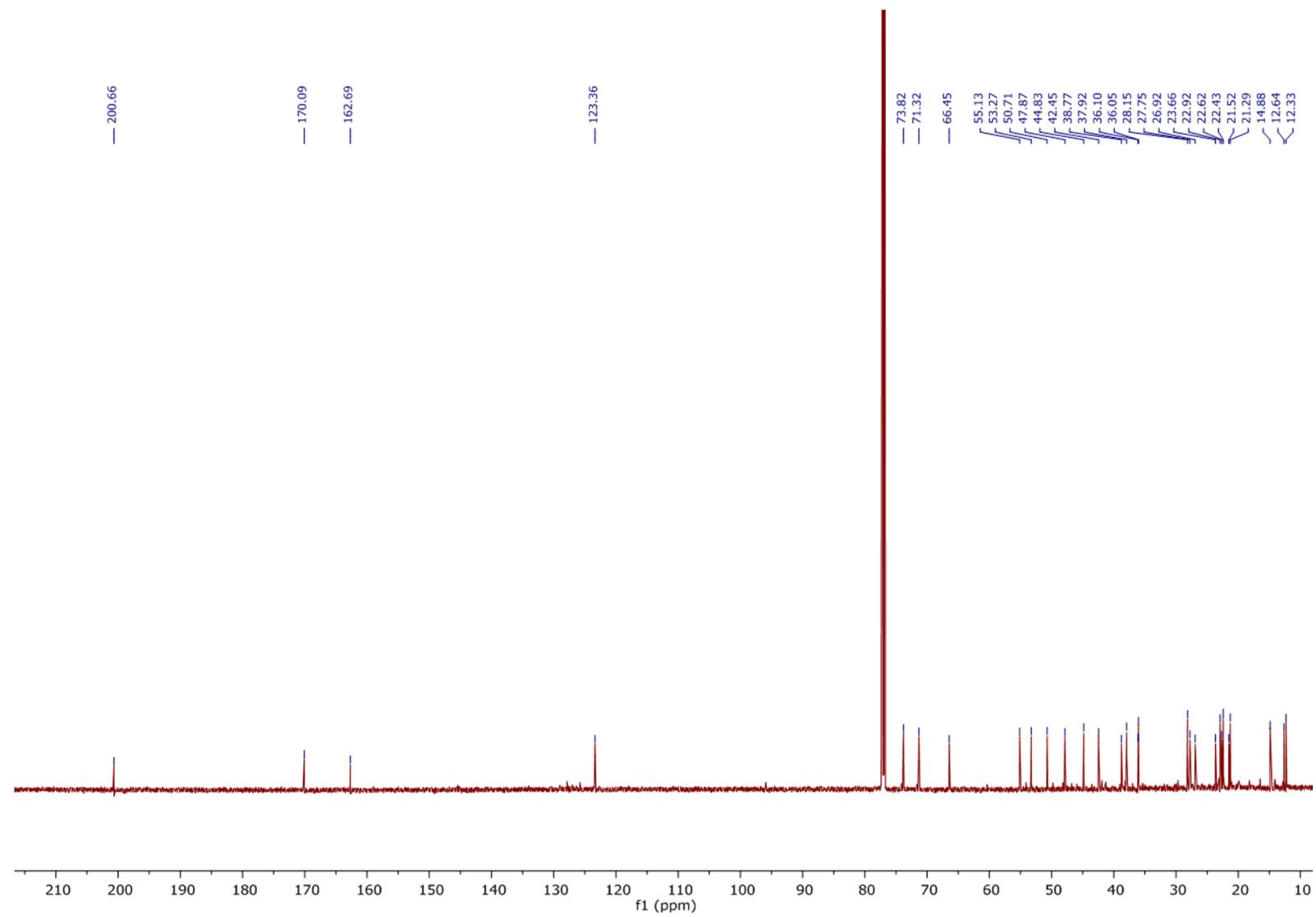


Figure S50. ^{13}C -NMR spectrum (150MHz, CDCl_3 , 303K) of compound 10

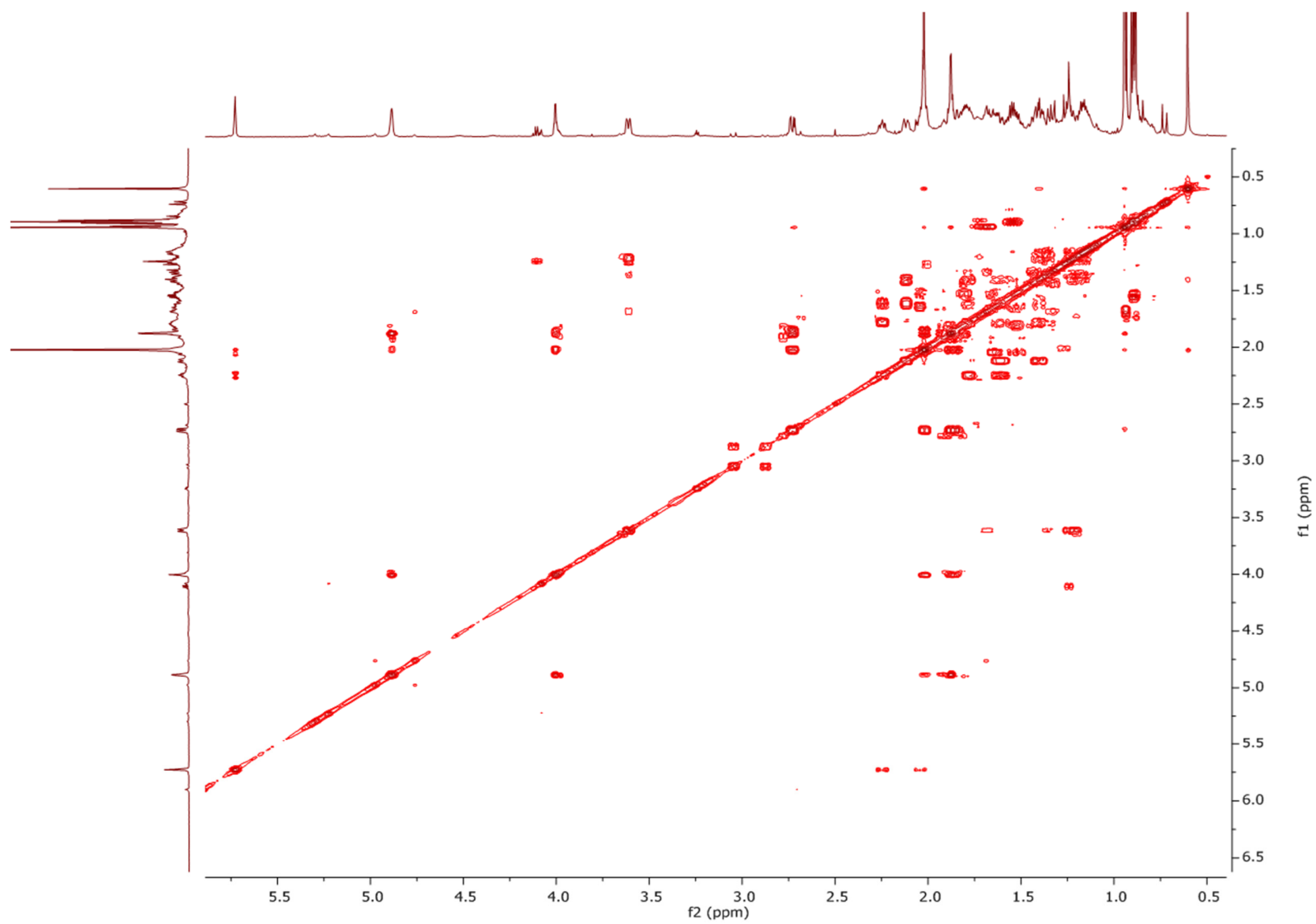


Figure S51. ^1H - ^1H COSY NMR spectrum (600MHz, CDCl_3 , 303K) of compound **10**

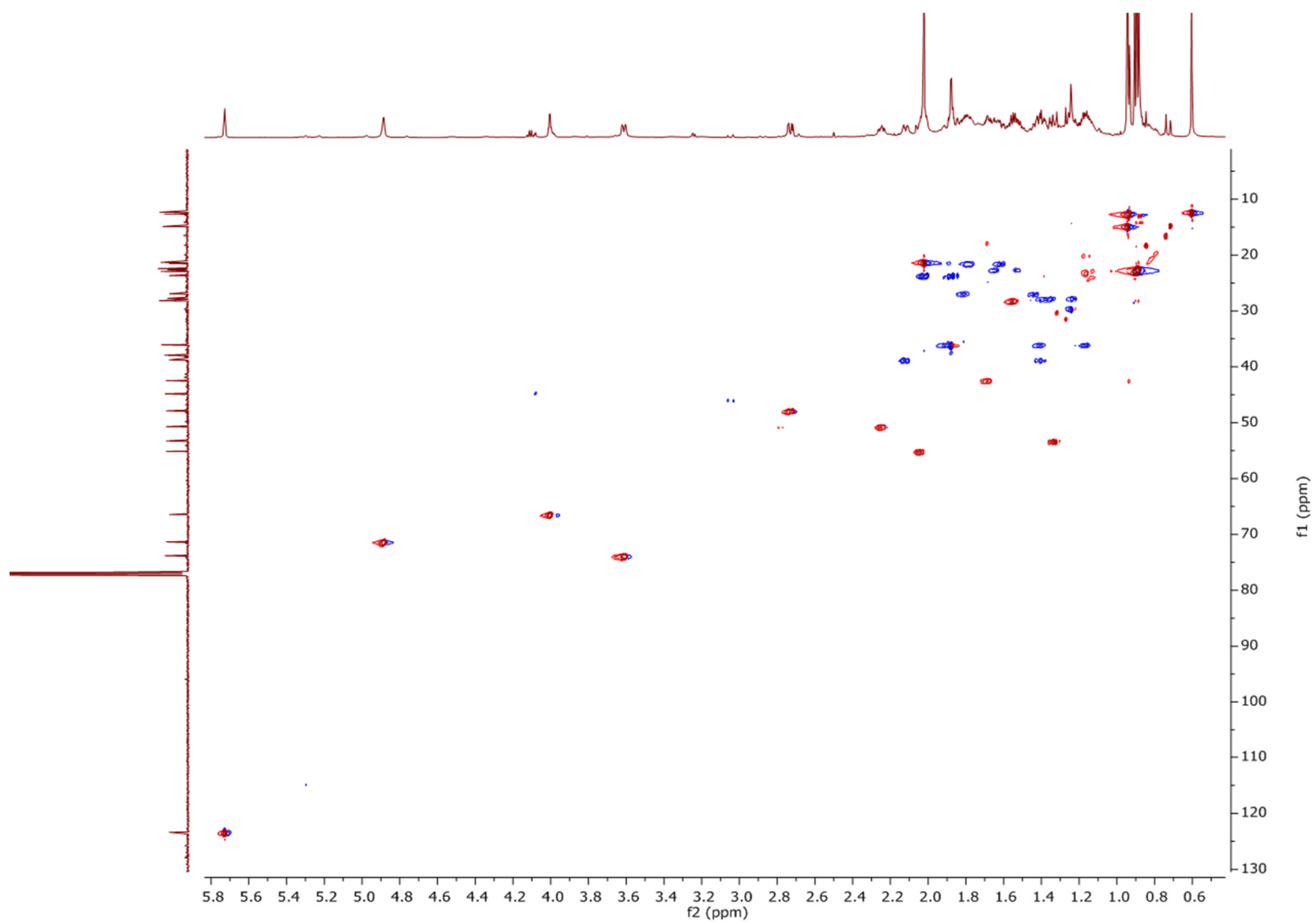


Figure S52. HSQC-DEPT NMR spectrum (600MHz, CDCl₃, 303K) of compound 10

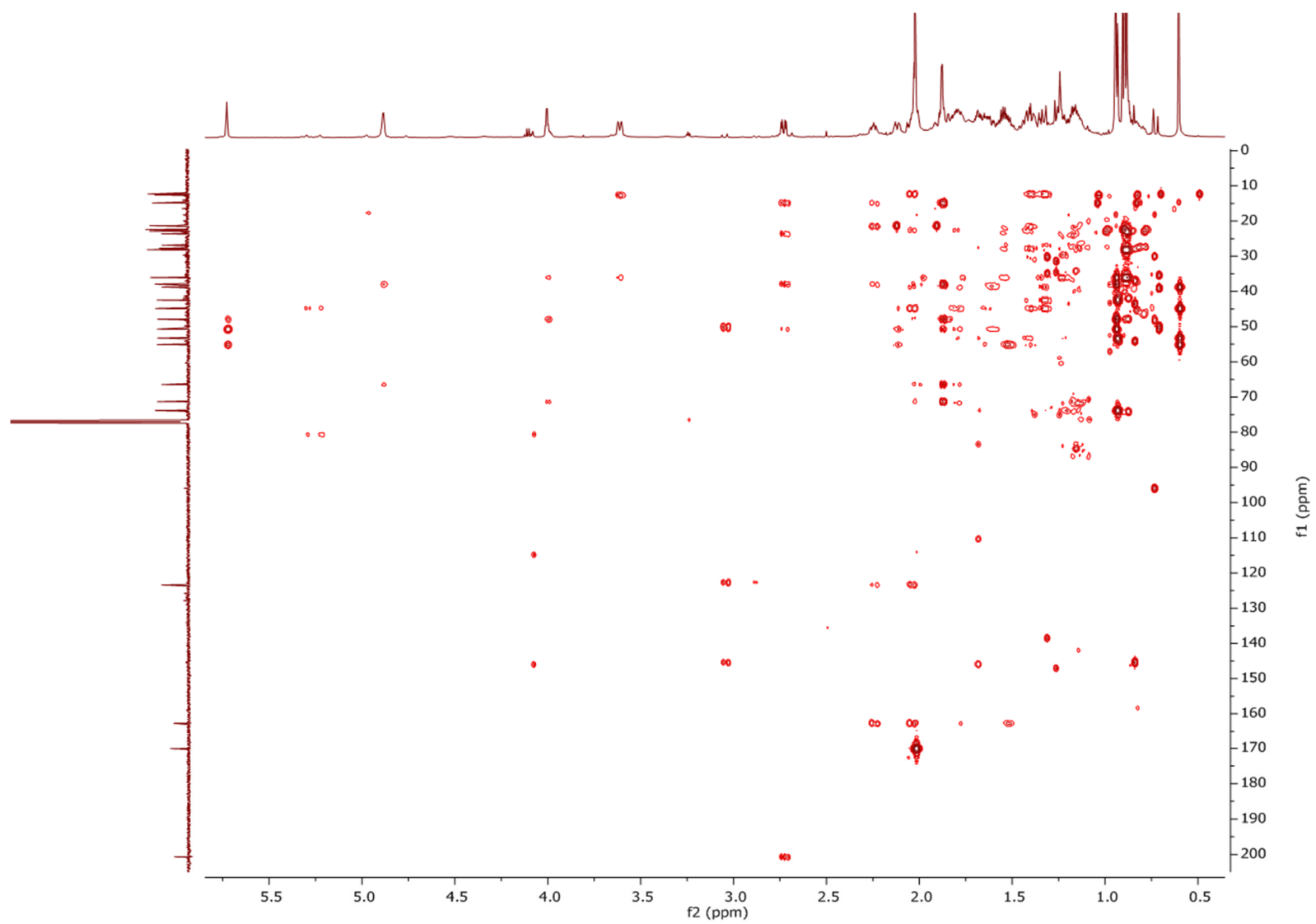


Figure S53. HMBC NMR spectrum (600MHz, CDCl₃, 303K) of compound 10

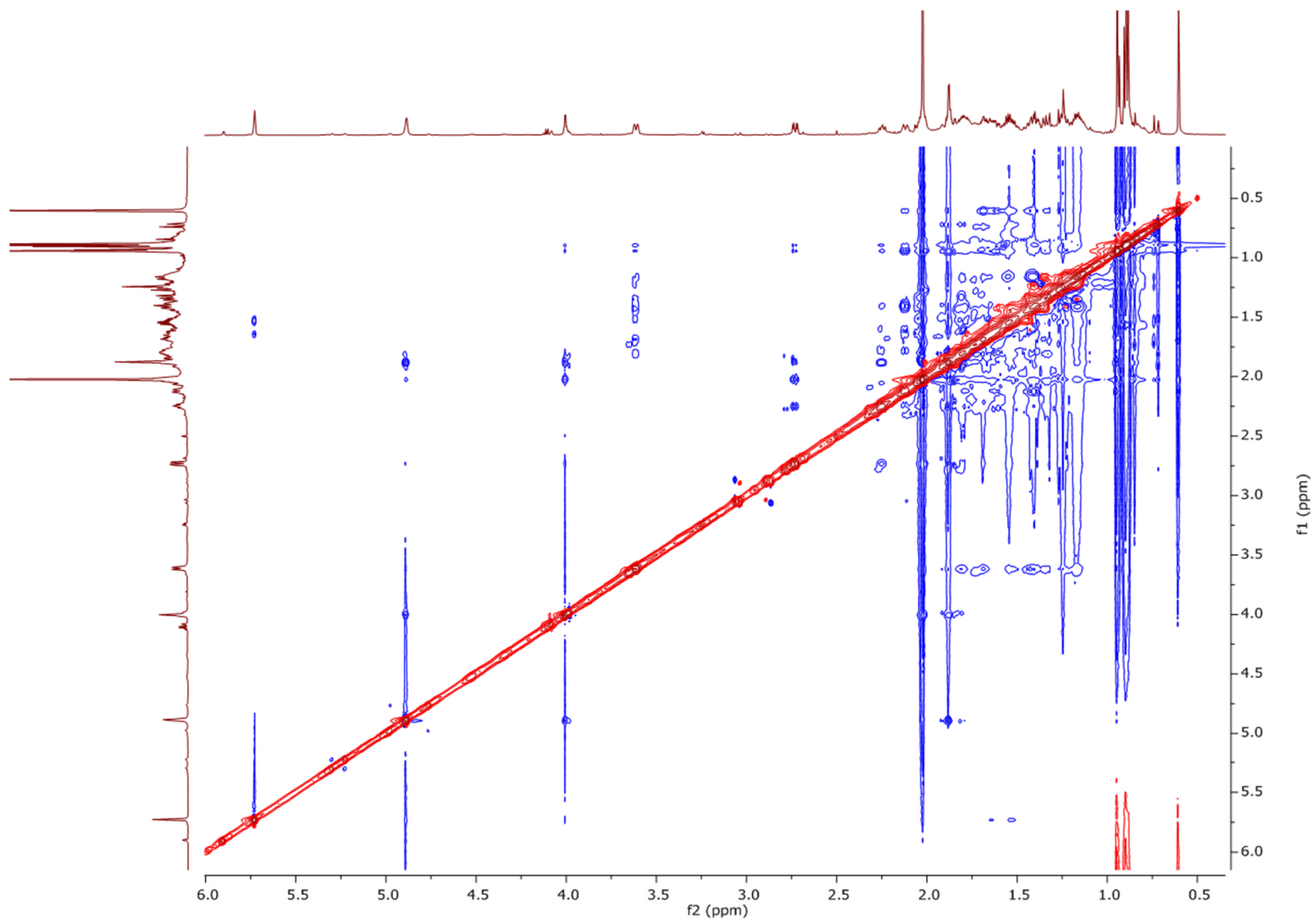


Figure S54. ROESY NMR spectrum (600MHz, CDCl₃, 303K) of compound 10

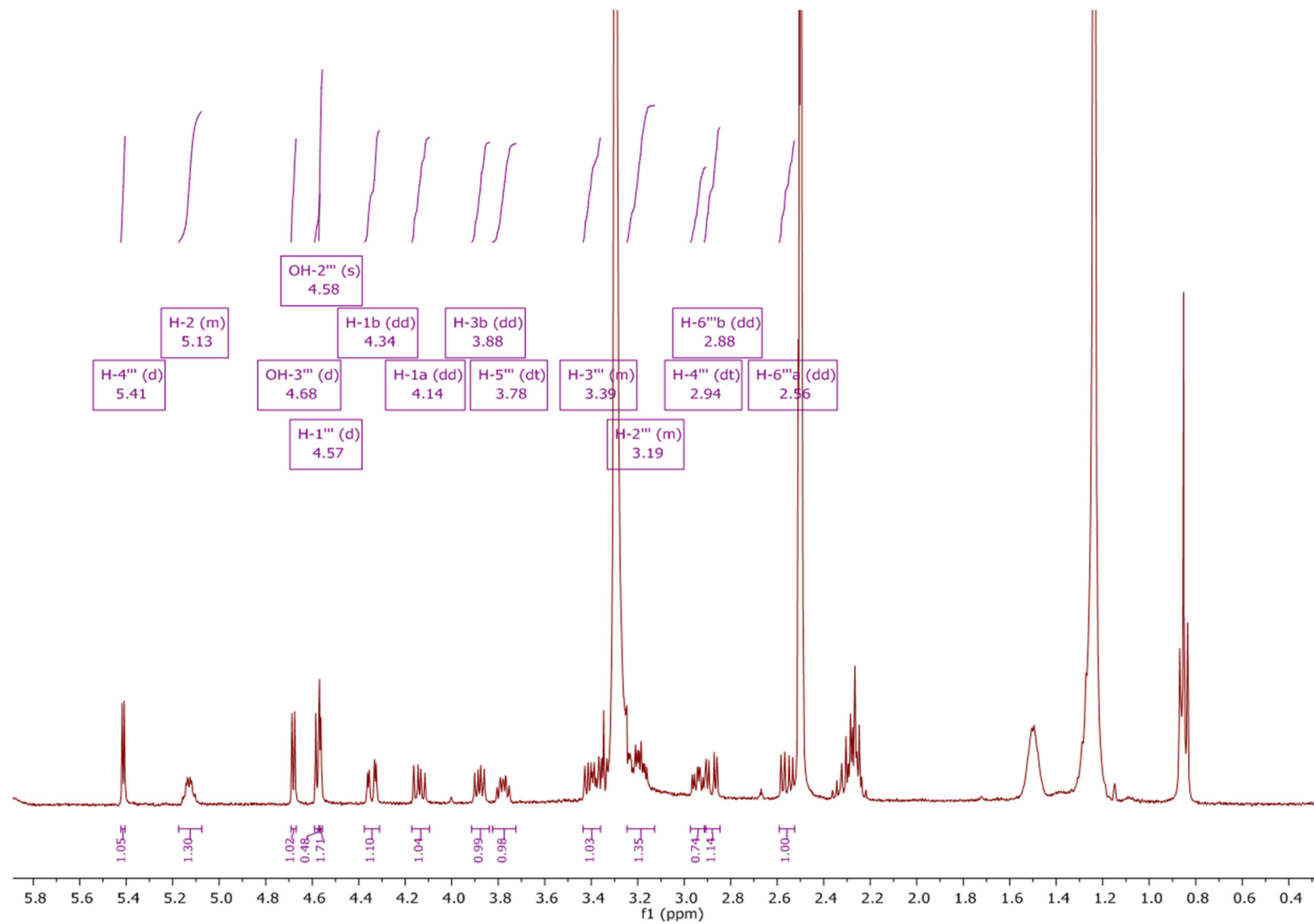


Figure S55. ¹H-NMR spectrum (600MHz, DMSO-d₆, 303K) of compound 11

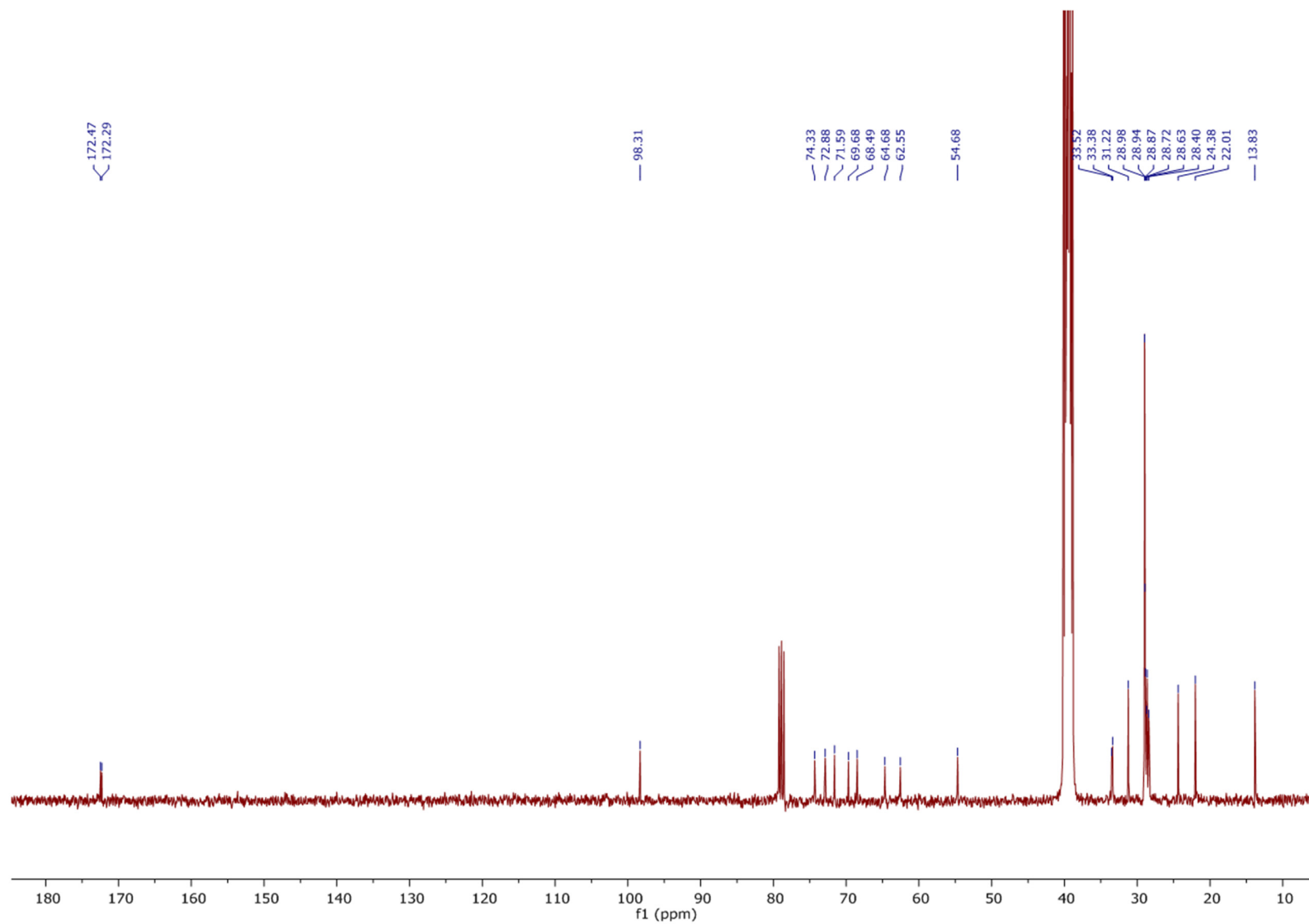


Figure S56. ^{13}C -NMR spectrum (150MHz, DMSO- d_6 , 303K) of compound 11

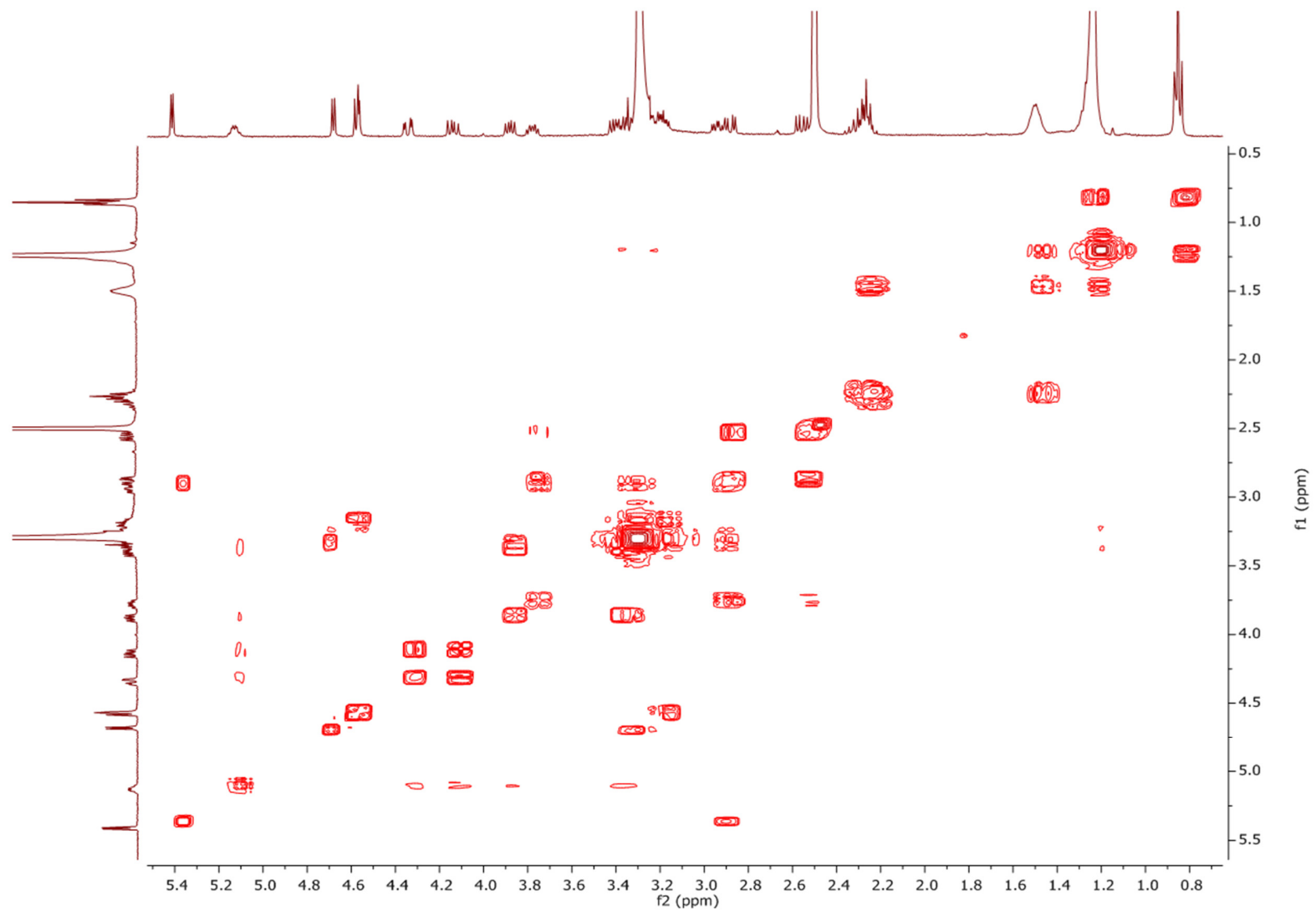


Figure S57. ^1H - ^1H COSY NMR spectrum (600MHz, DMSO- d_6 , 303K) of compound 11

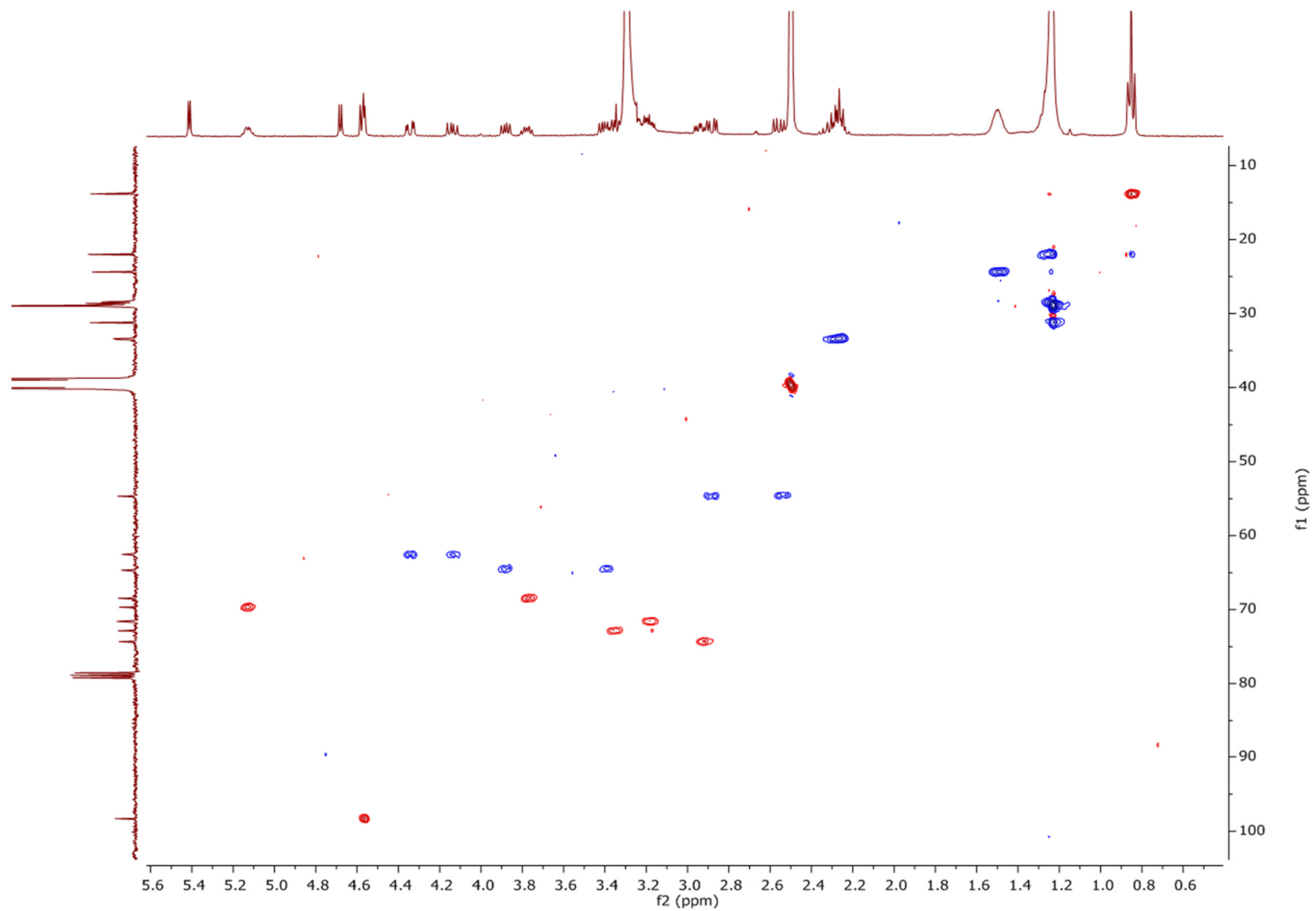


Figure S58. HSQC-DEPT NMR spectrum (600MHz, DMSO-d₆, 303K) of compound **11**

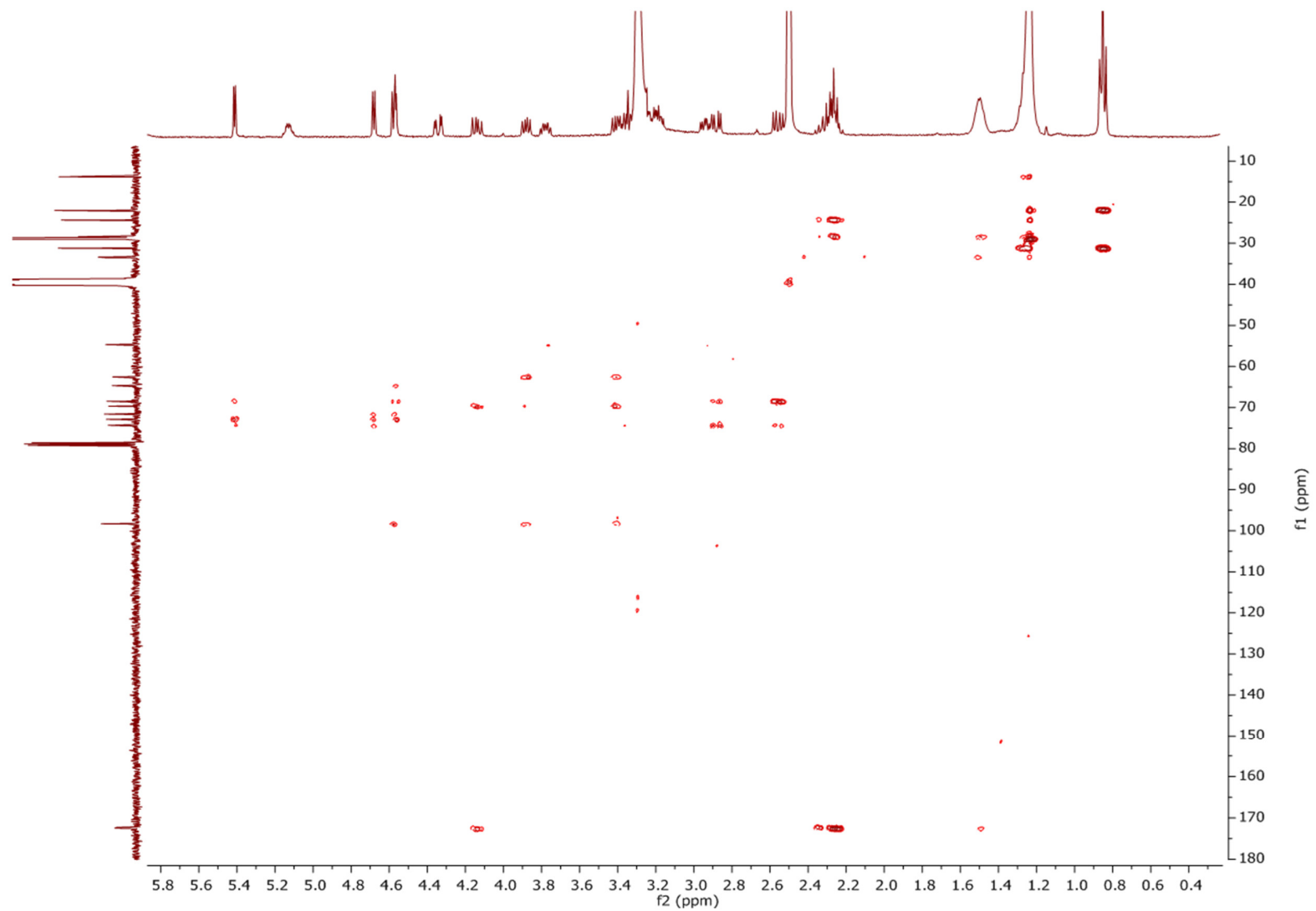


Figure S59. HMBC NMR spectrum (600MHz, DMSO-d₆, 303K) of compound **11**

1: TOF MS ES+
2.51e4

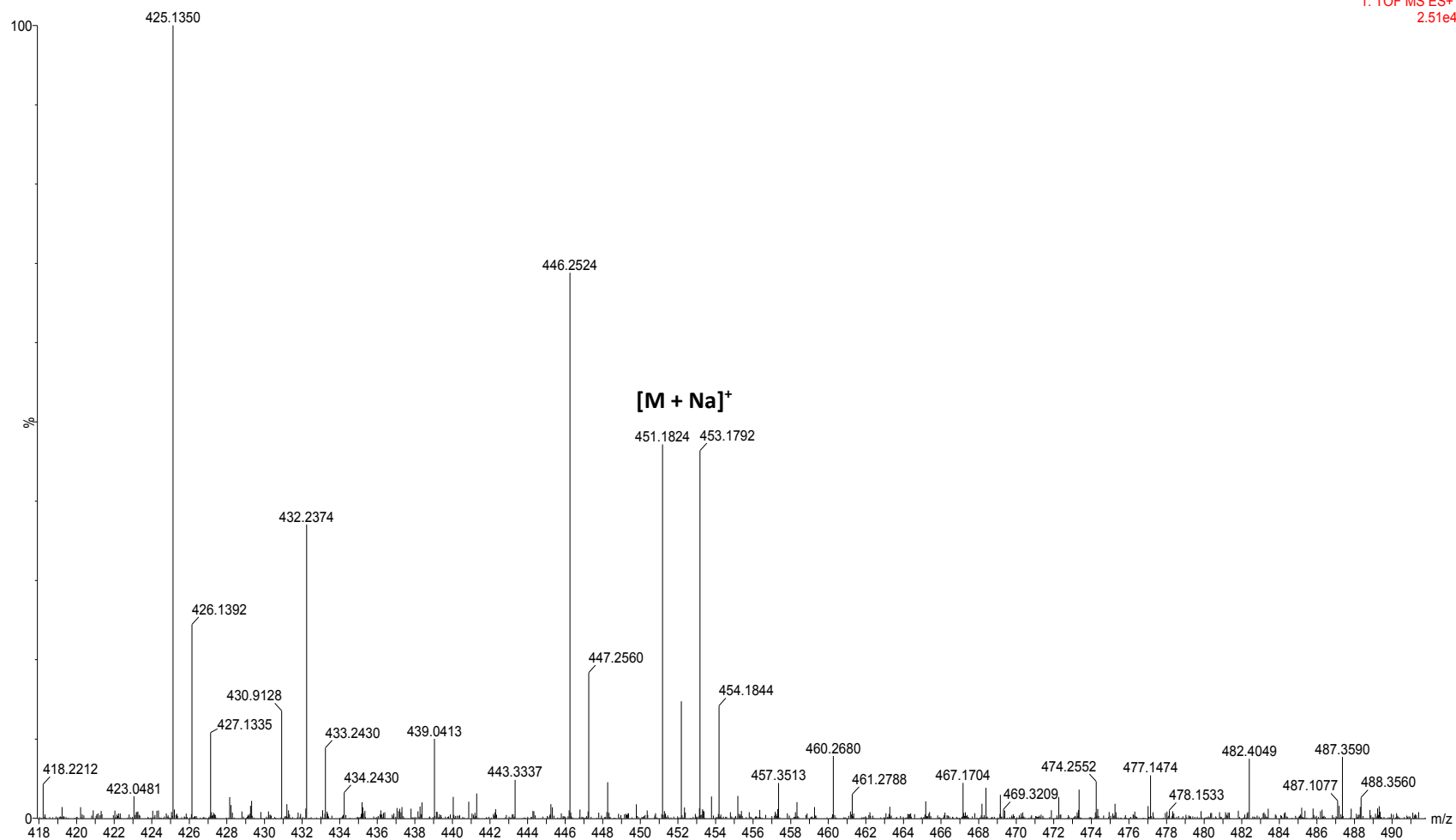


Figure S60. HR-ESI-MS spectrum of compound 1

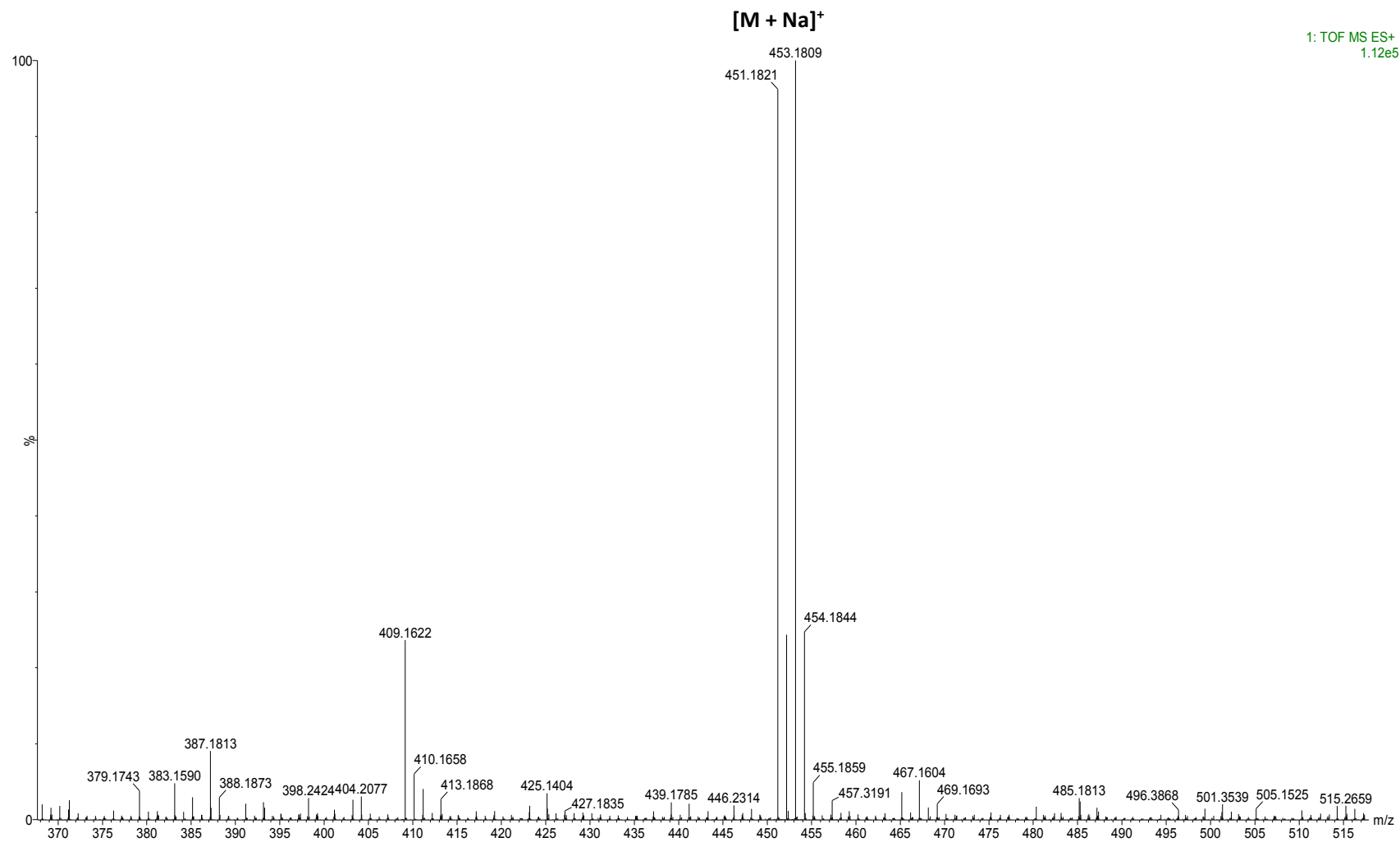


Figure S61. HR-ESI-MS spectrum of compound 2

1: TOF MS ES+
1.12e5

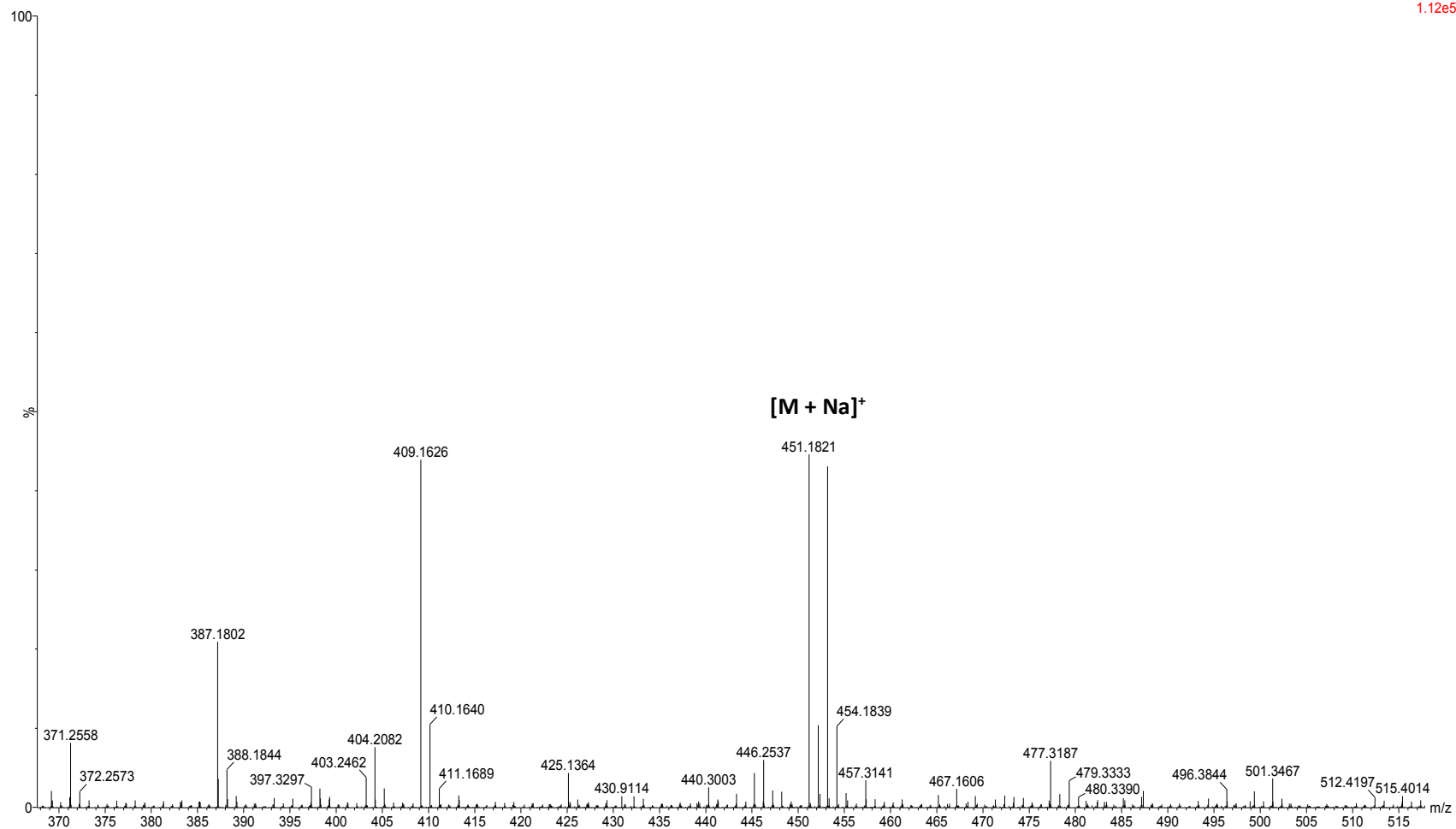


Figure S62. HR-ESI-MS spectrum of compound 3

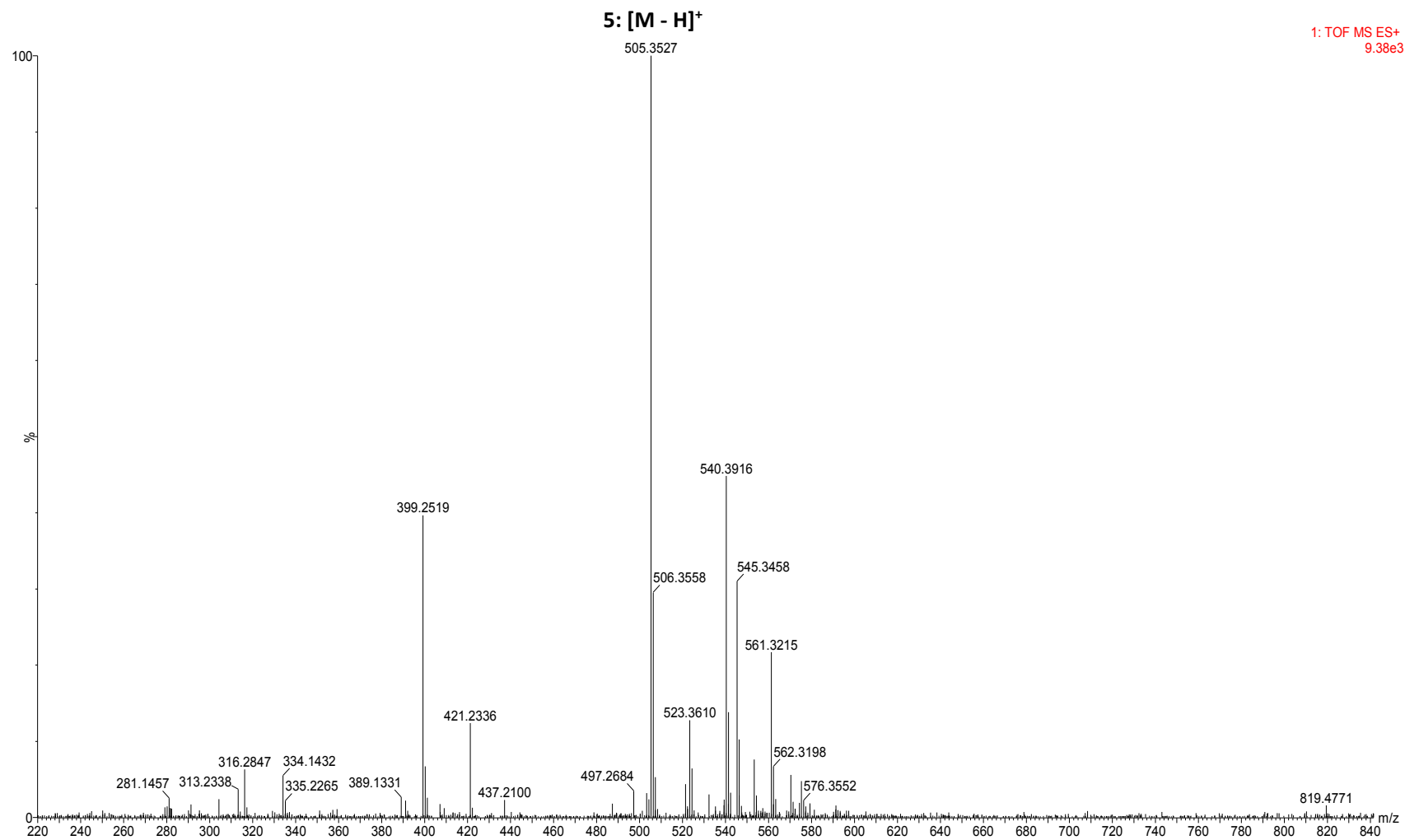


Figure S63. HR-ESI-MS spectrum of compound 5

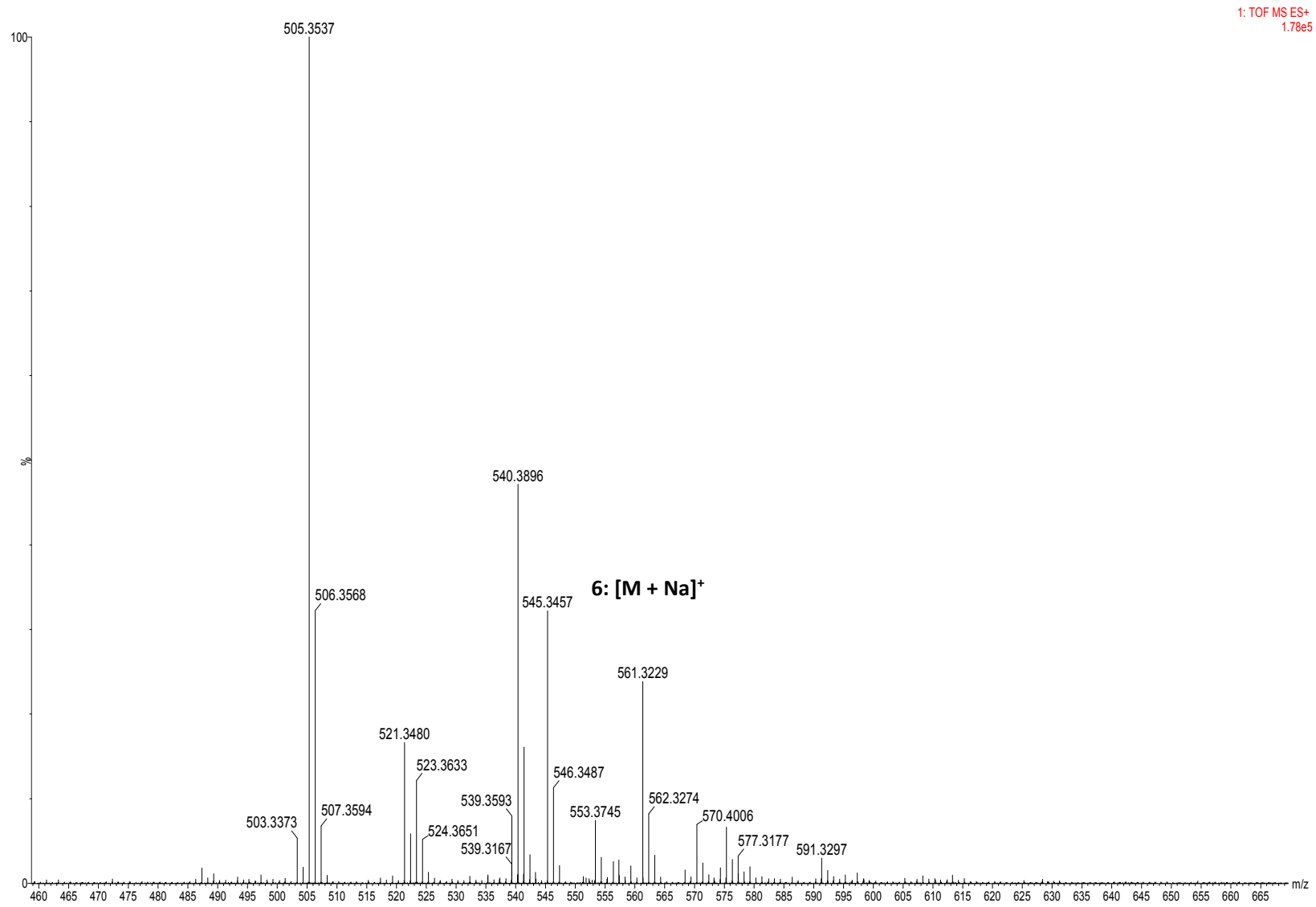


Figure S64. HR-ESI-MS spectrum of compound 6

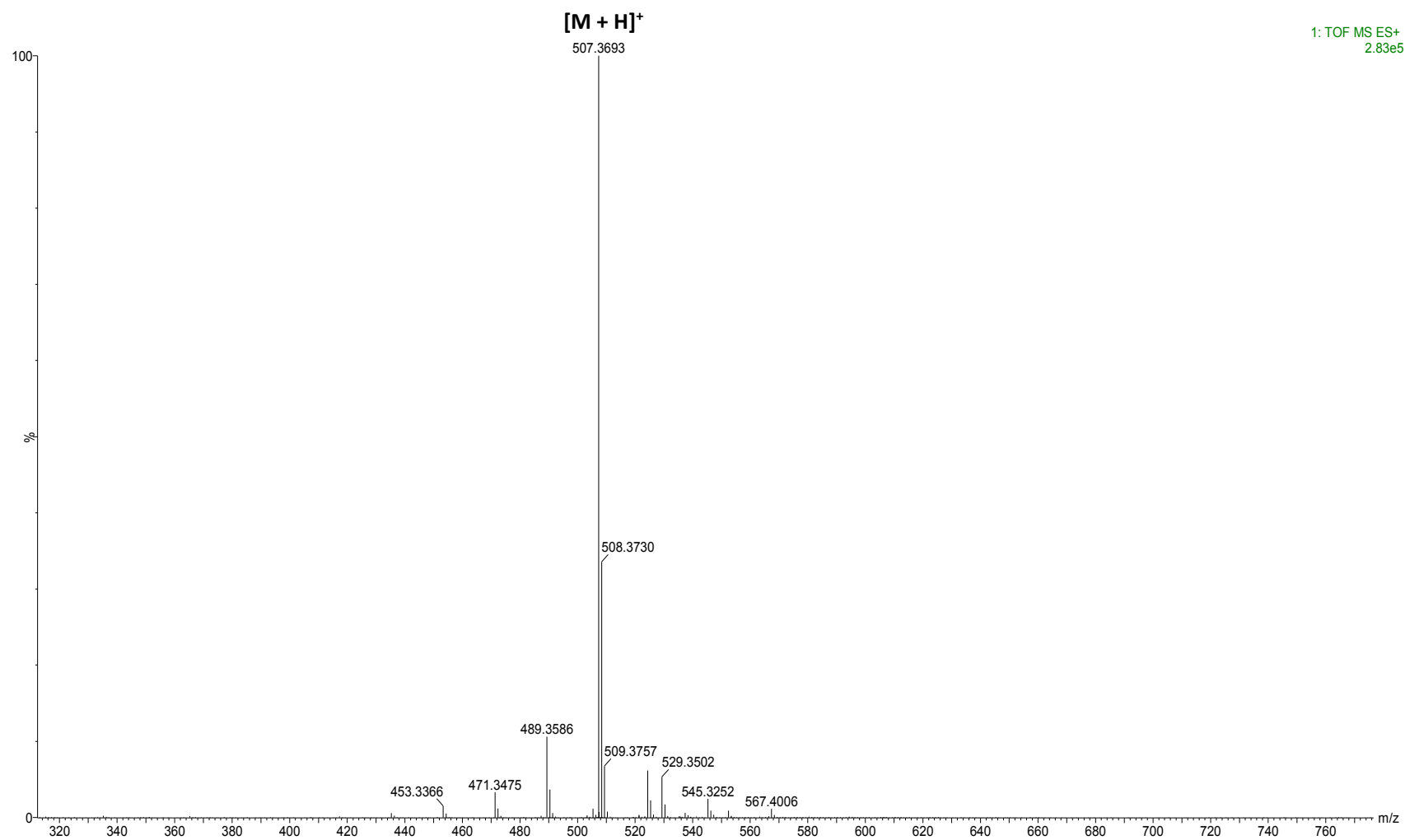


Figure S65. HR-ESI-MS spectrum of compound 7

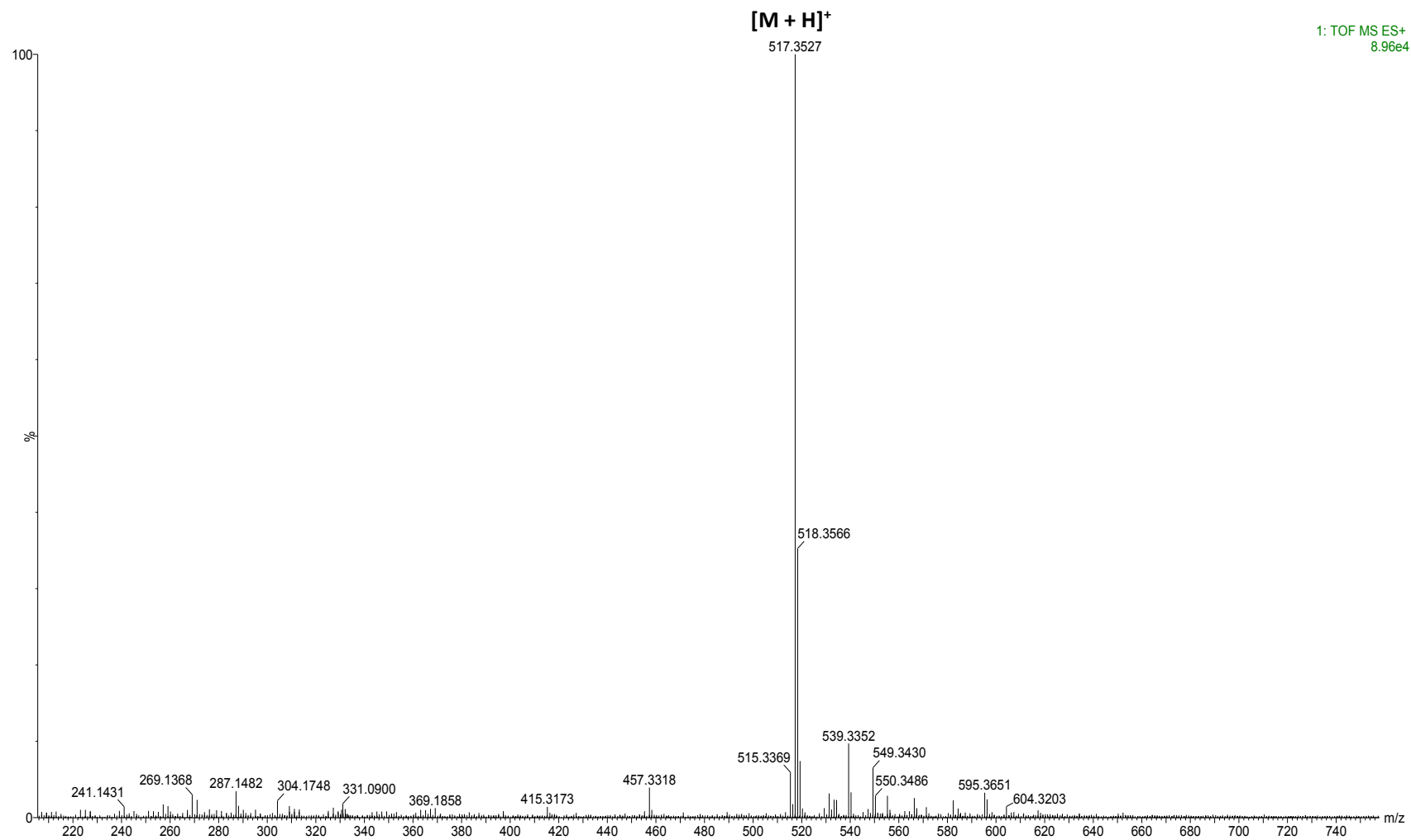


Figure S66. HR-ESI-MS spectrum of compound 8

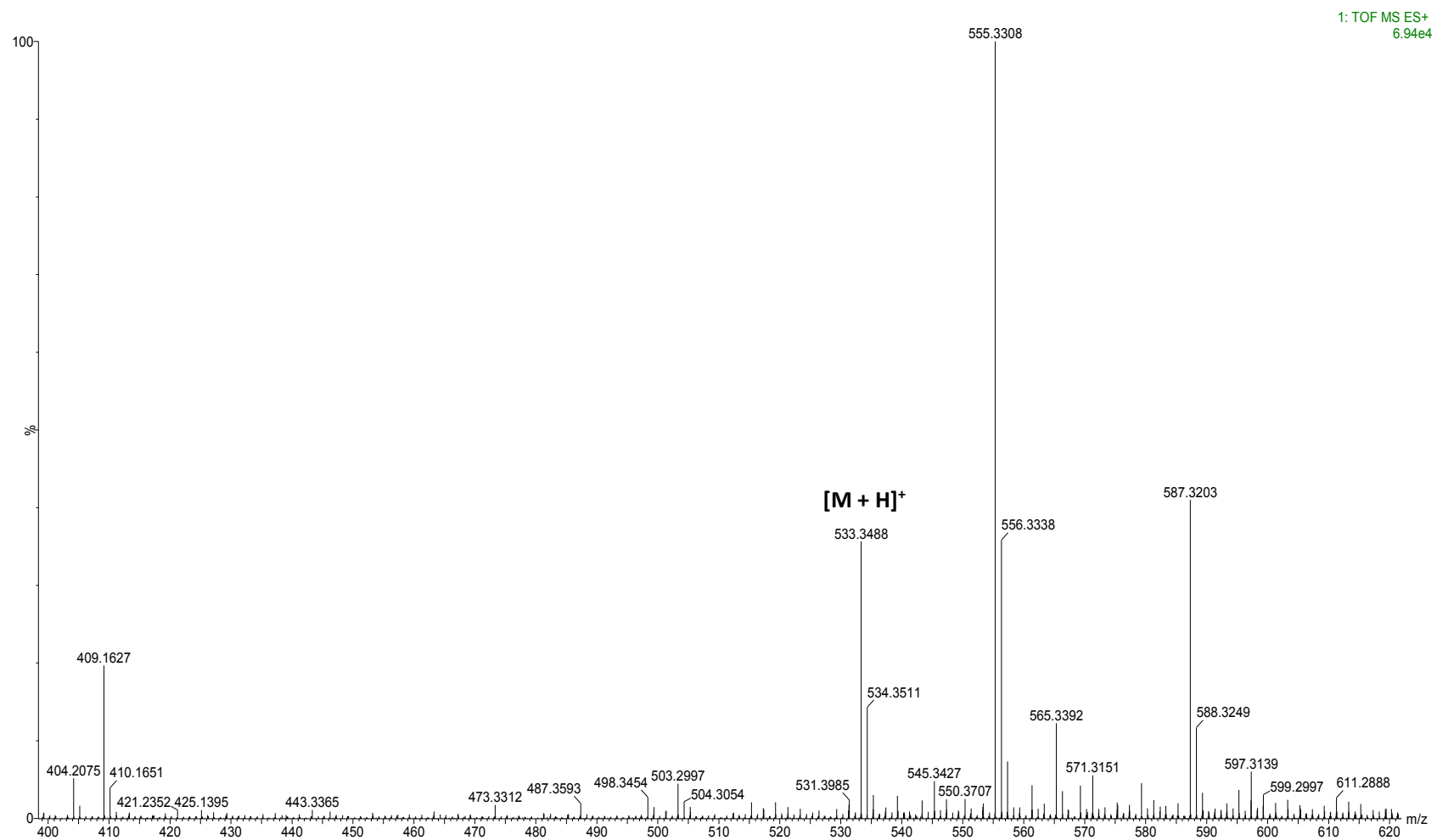


Figure S67. HR-ESI-MS spectrum of compound 9

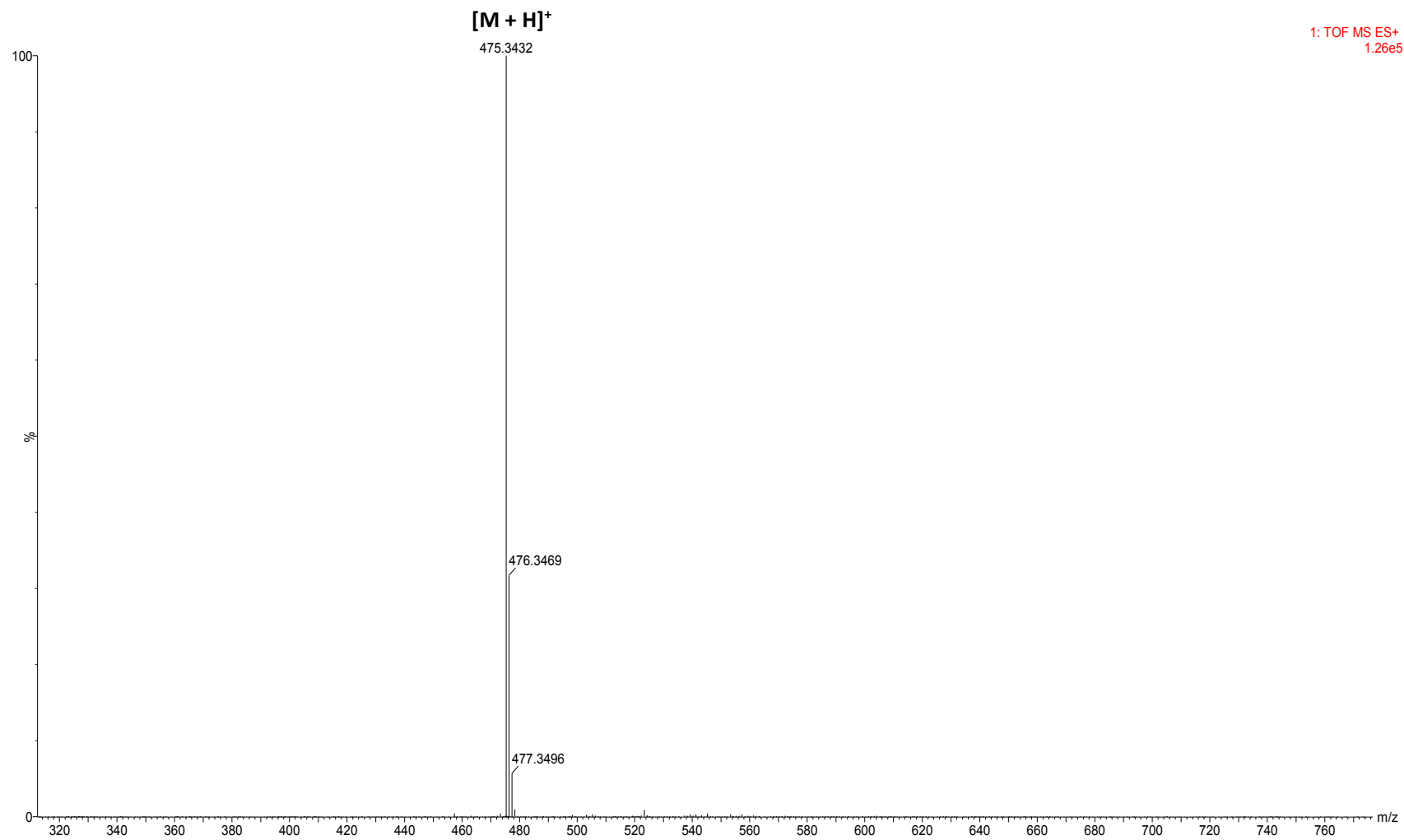


Figure S68. HR-ESI-MS spectrum of compound 10

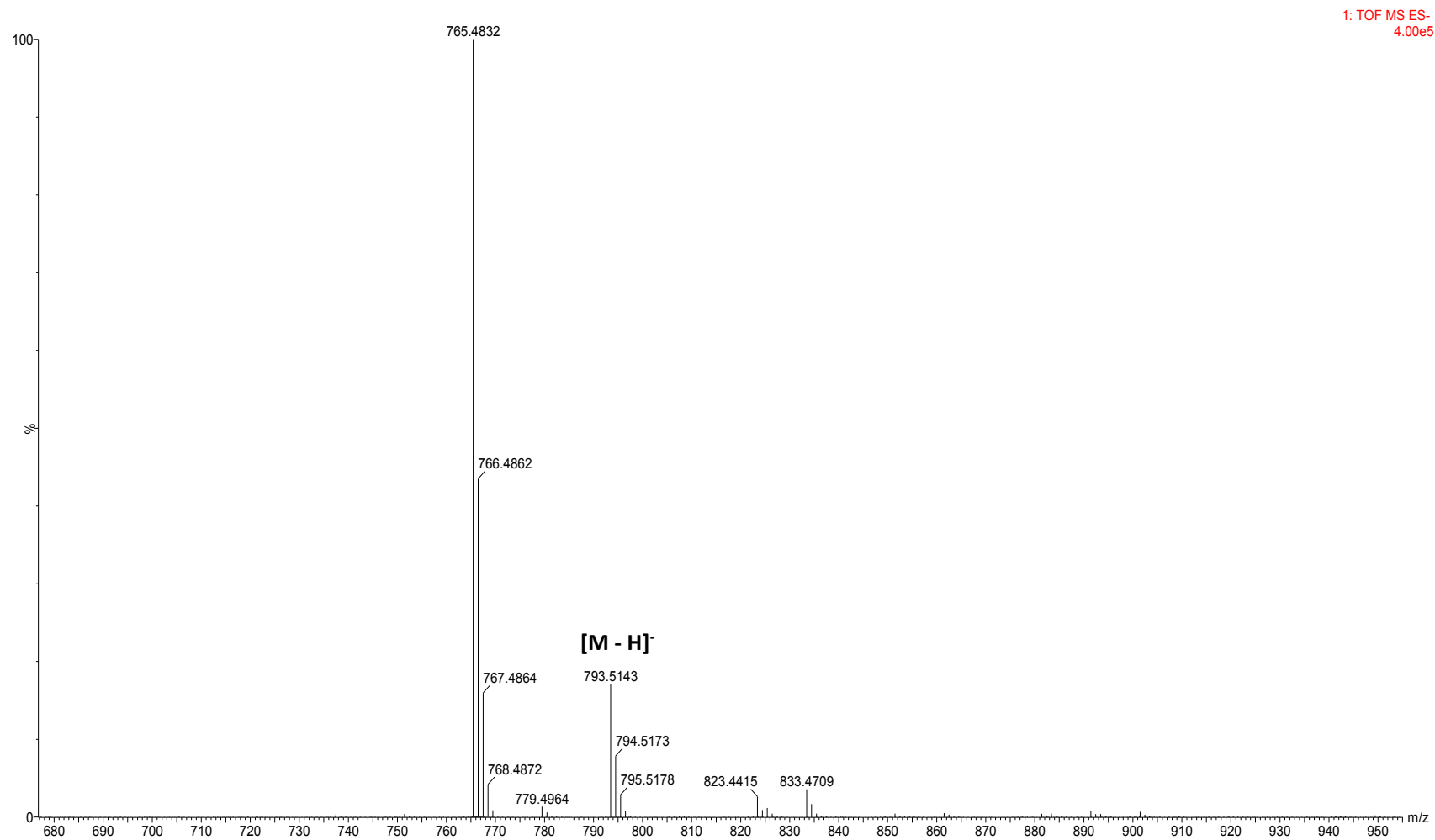


Figure S69. HR-ESI-MS spectrum of compound 11

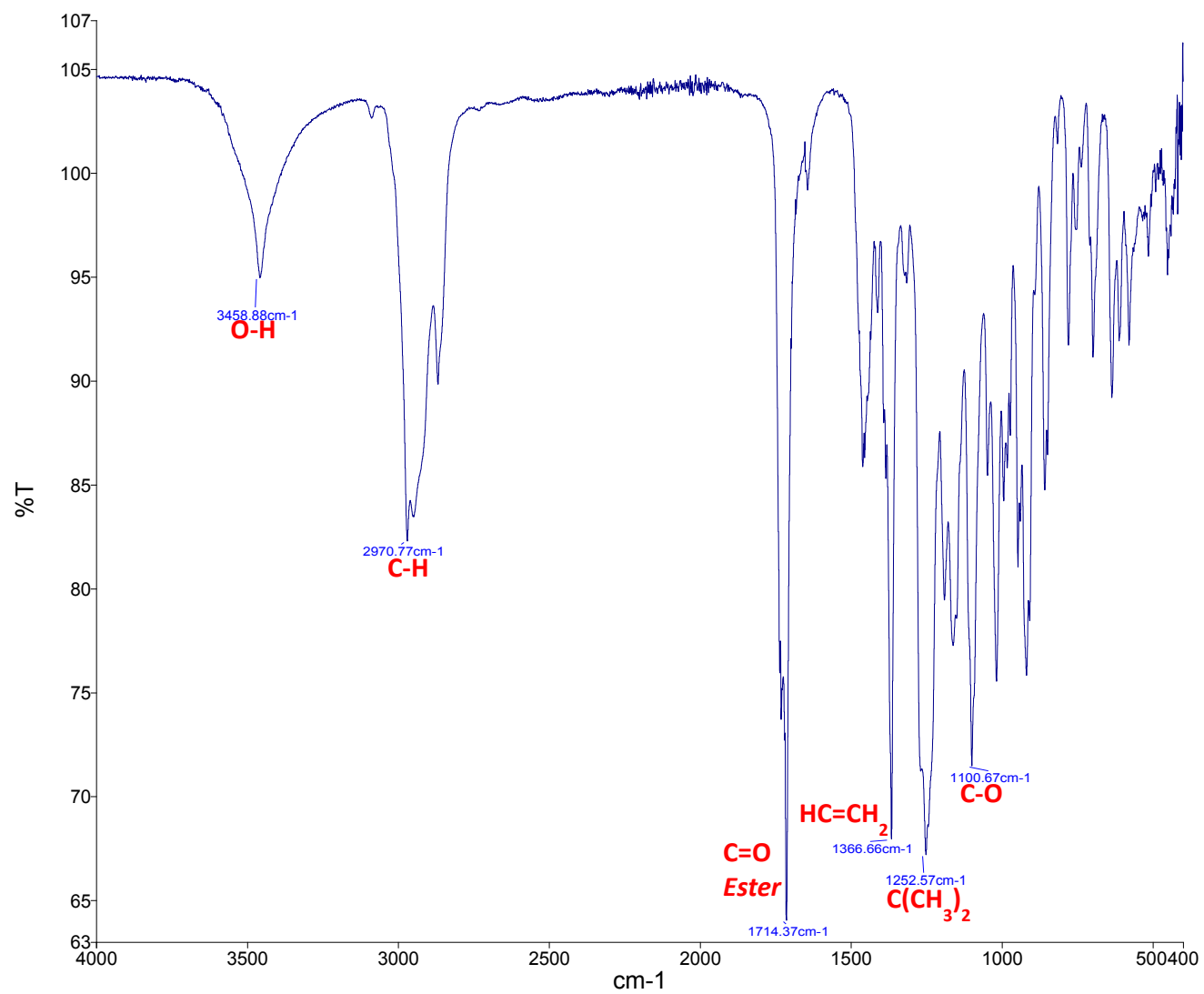


Figure S70. IR spectrum of compound 1

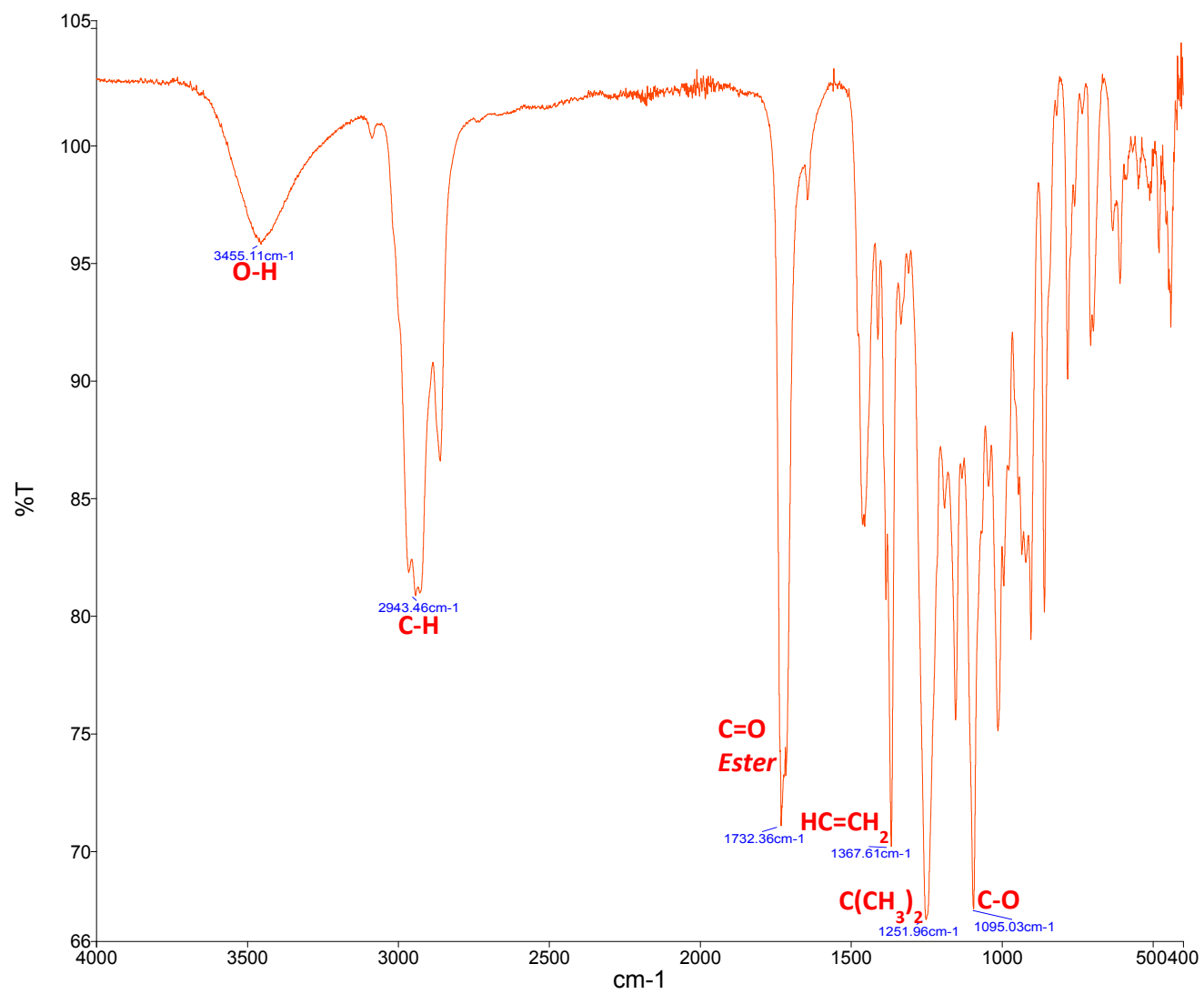


Figure S71. IR spectrum of compound 2

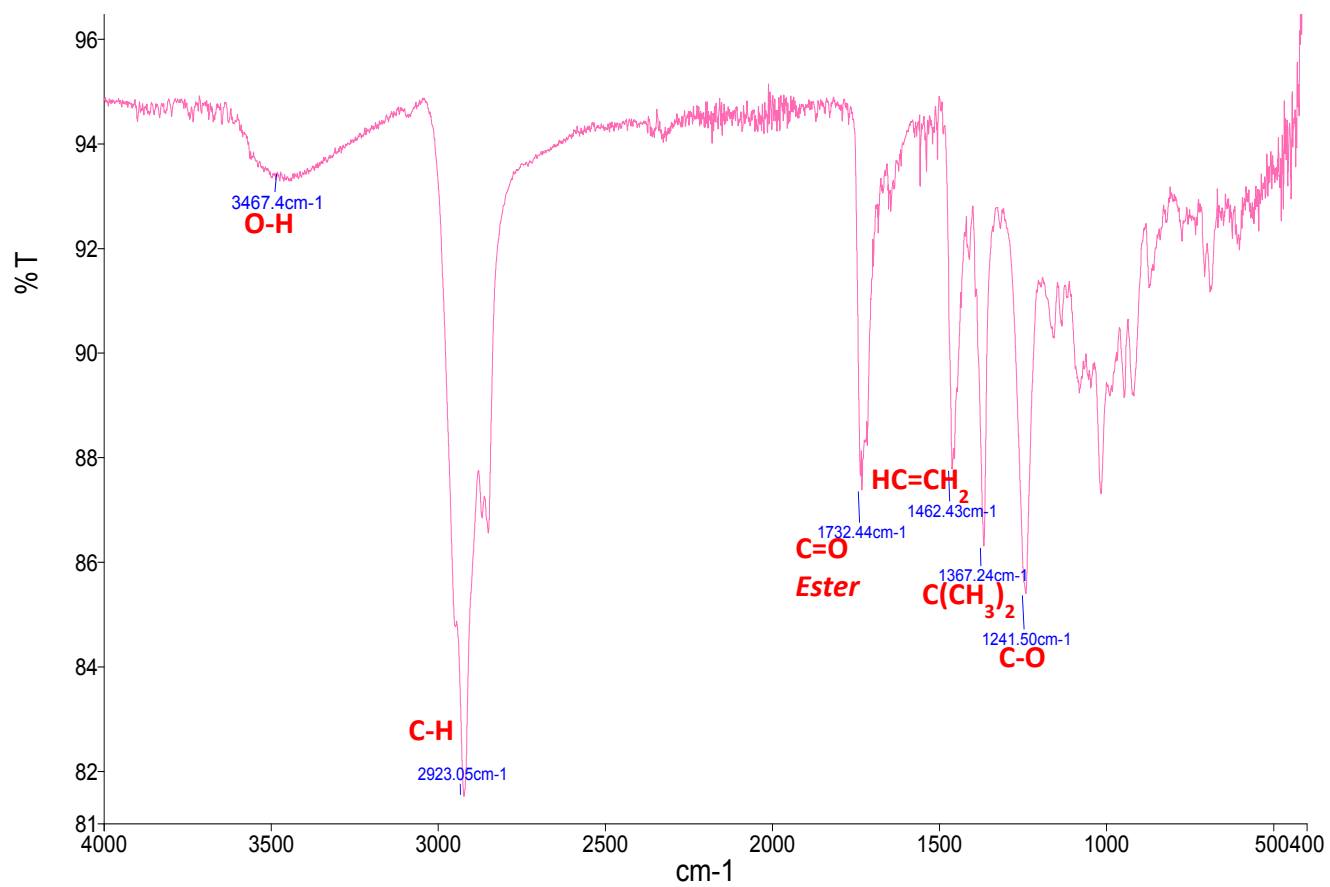


Figure S72. IR spectrum of compound 3

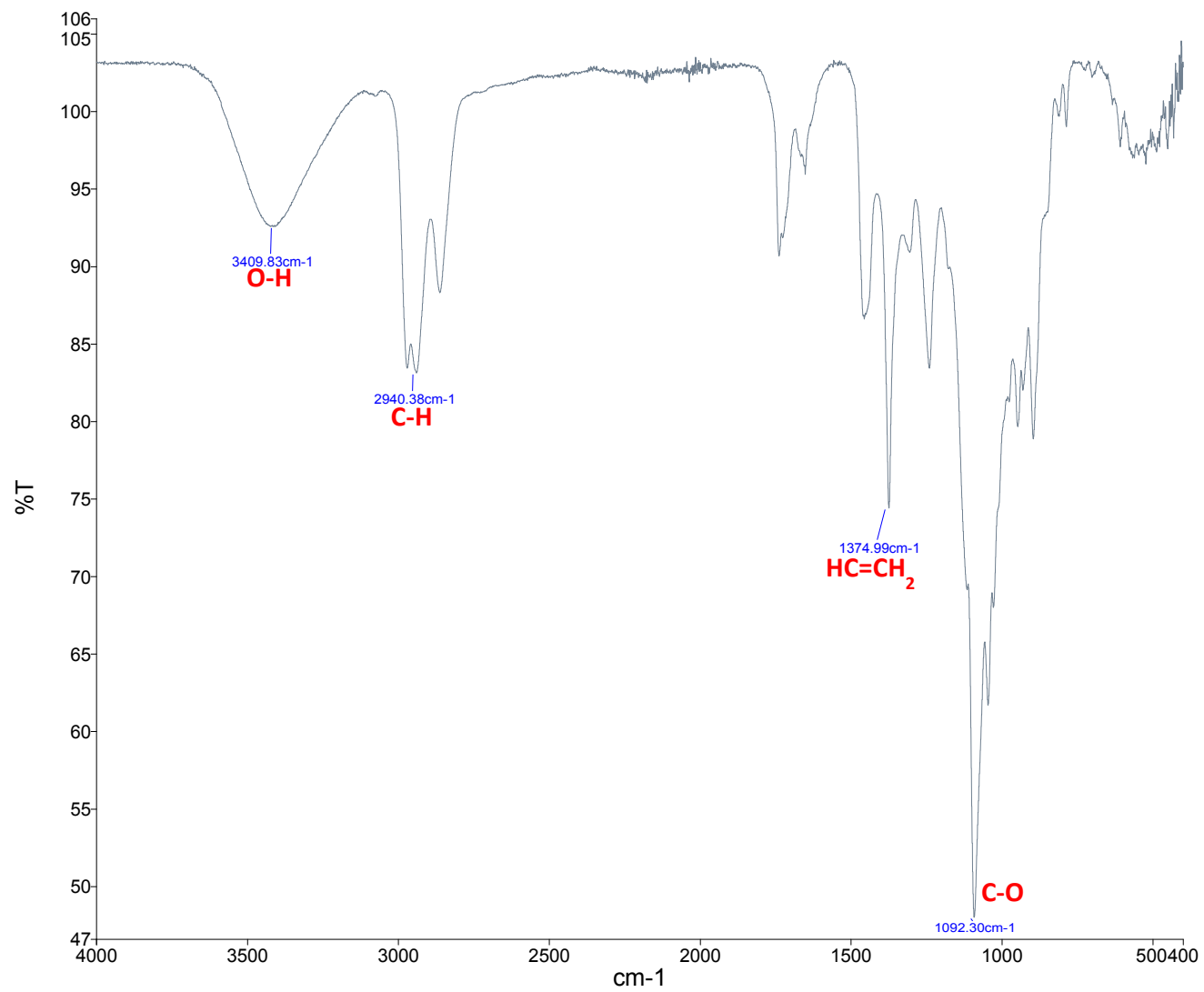


Figure S73. IR spectrum of compound 7

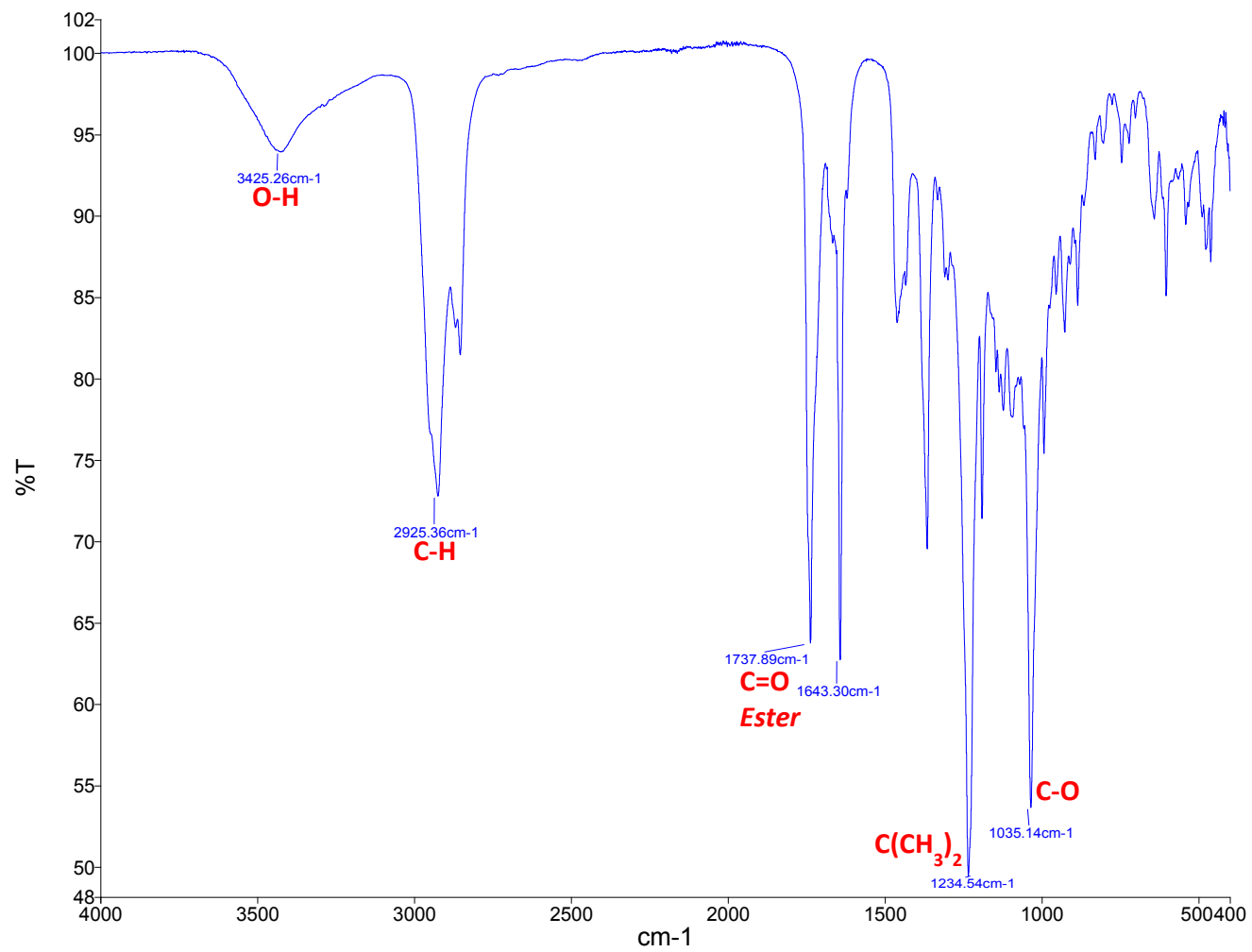


Figure S74. IR spectrum of compound 8

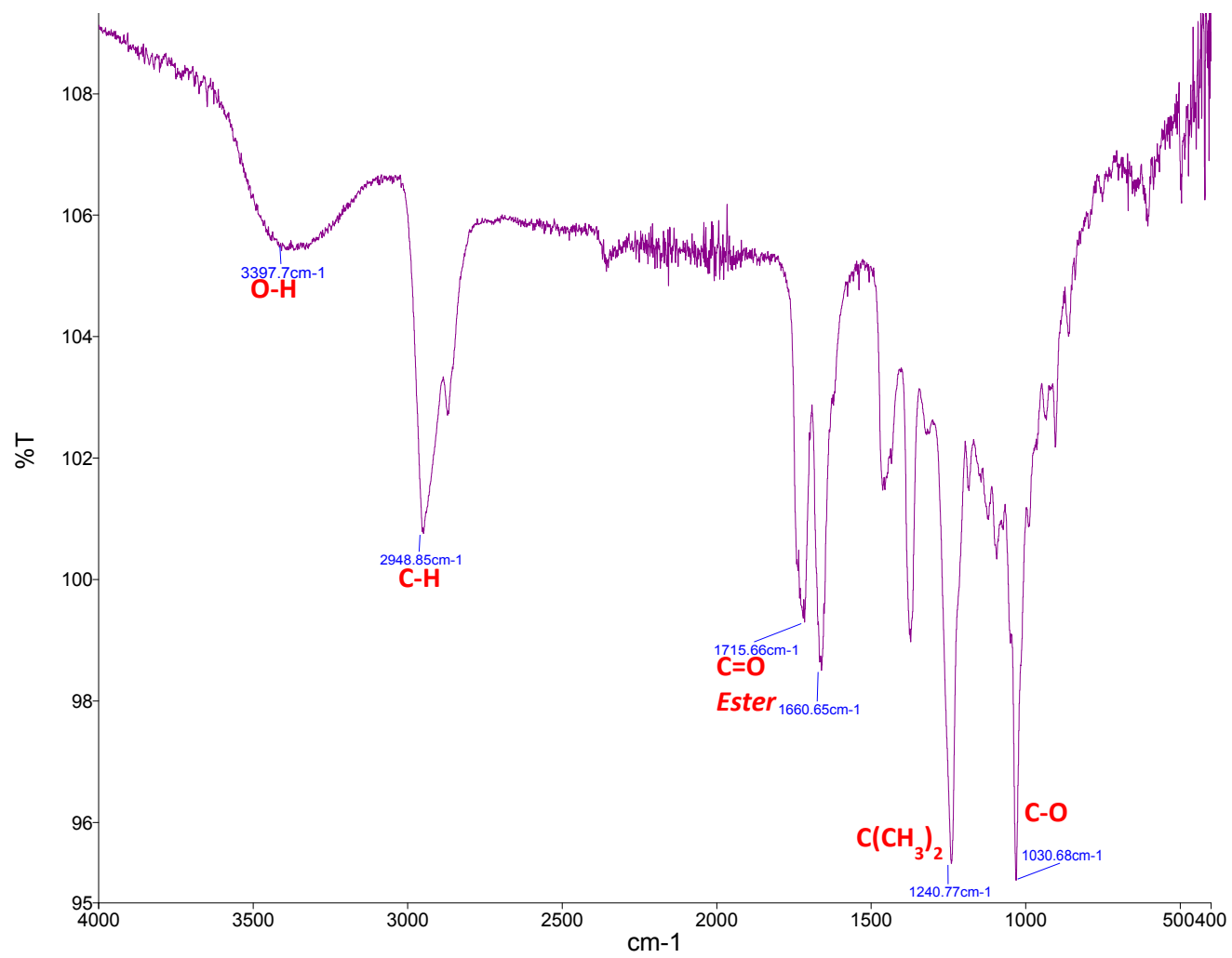


Figure S75. IR spectrum of compound 10

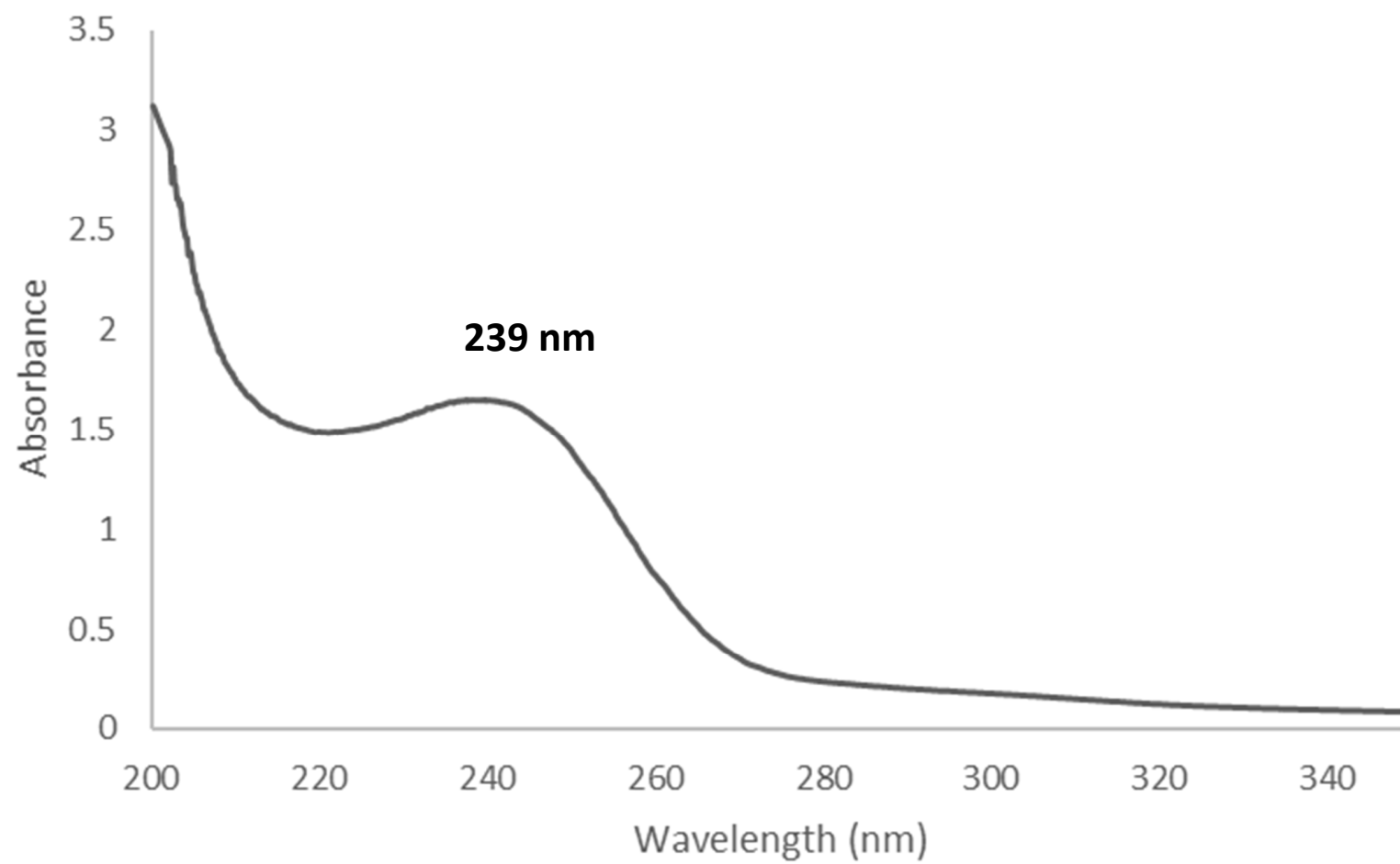


Figure S76. UV spectrum of compound 8

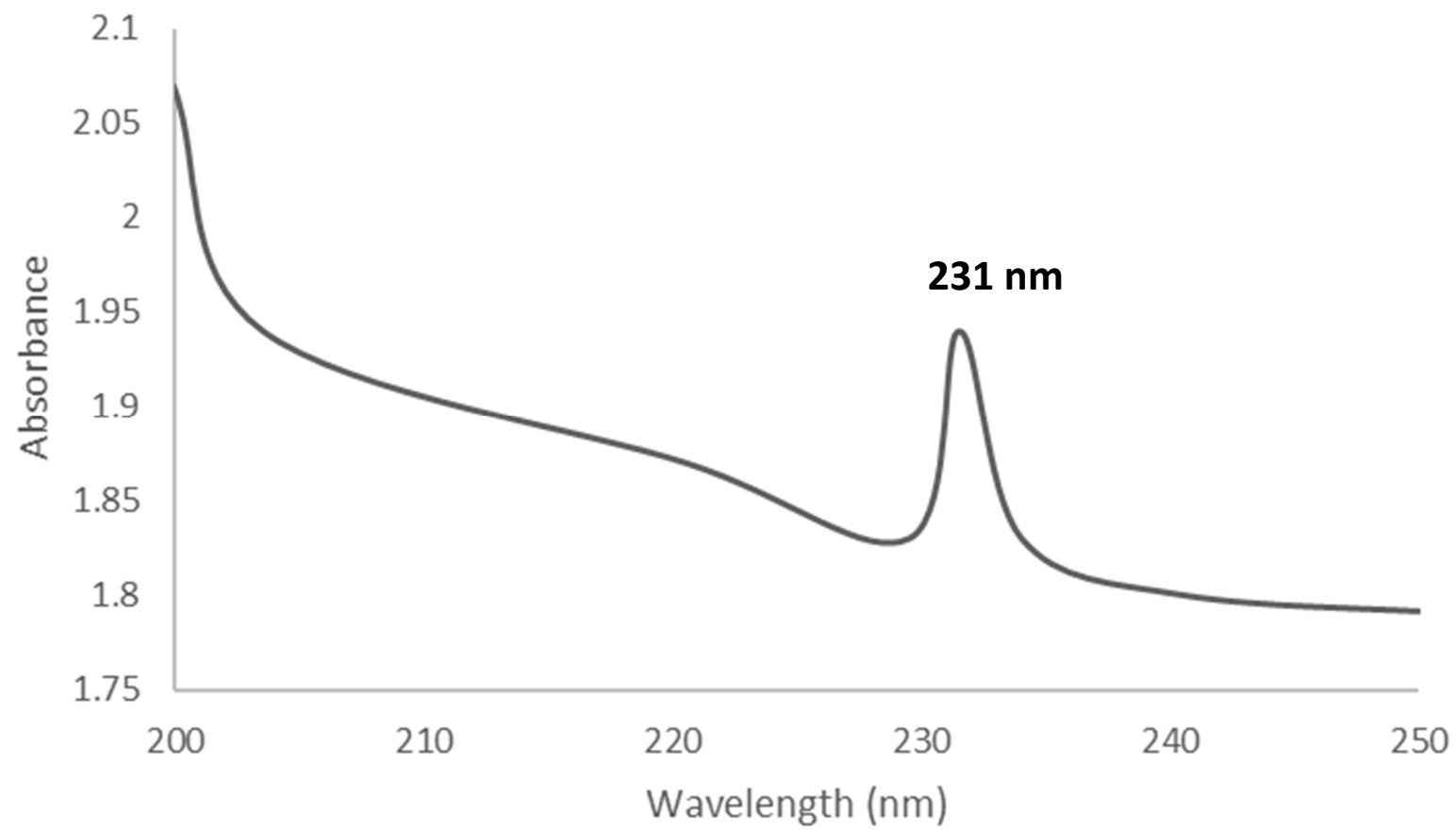


Figure S77. UV spectrum of compound **10**

Table S1. Cytotoxicity assay data for compounds **1 - 10**

Compound	MDA-MB-231			HeLa		
	IC₅₀ (μM)	SEM	R²	IC₅₀ (μM)	SEM	R²
1	26.3	1	0.9952	30.2	1.2	0.9309
2	53.7	1.2	0.8924	9.3	1.3	0.9215
3	58.5	1.3	0.9756	42	1.2	0.9346
4	44.4	1.1	0.9812	21.1	1.1	0.9584
5 + 6	13.5	1.1	0.9883	46.4	1.1	0.9822
7	8.8	5.6	0.9913	133.8	1.1	0.9716
8	27.6	1.1	0.9748	25.6	1.2	0.9304
9	15.8	1.1	0.9907	48.2	3.3	0.9732
10	21.6	1.1	0.9797	43.5	1.2	0.9213