

Electronic Supplementary Information
New Journal of Chemistry

Nucleoside bearing boron clusters and their phosphoramidites – building blocks for
modified oligonucleotide synthesis

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¹H-, ¹³C-, ¹¹B-, ¹¹B{H BB}-, ³¹P-NMR, DEPT-135, IR, MS spectra of 1,2-dicarba-*closo*-
dodecaborane derivatives of thymidine: **20**, **21**, **29**, 2'-deoxycytidine: **22**, **23**, **30**, 2'-
deoxyadenosine: **12-14**, **24**, **25**, **31**, 2'-deoxyguanosine: **16**, **17**, **26-28**, **32**, and conjugates
with opened-cage 7,8-dicarba-*nido*-undecaborate ion **33-36**. CD spectra for **20**, **22**, **24**, **27**,
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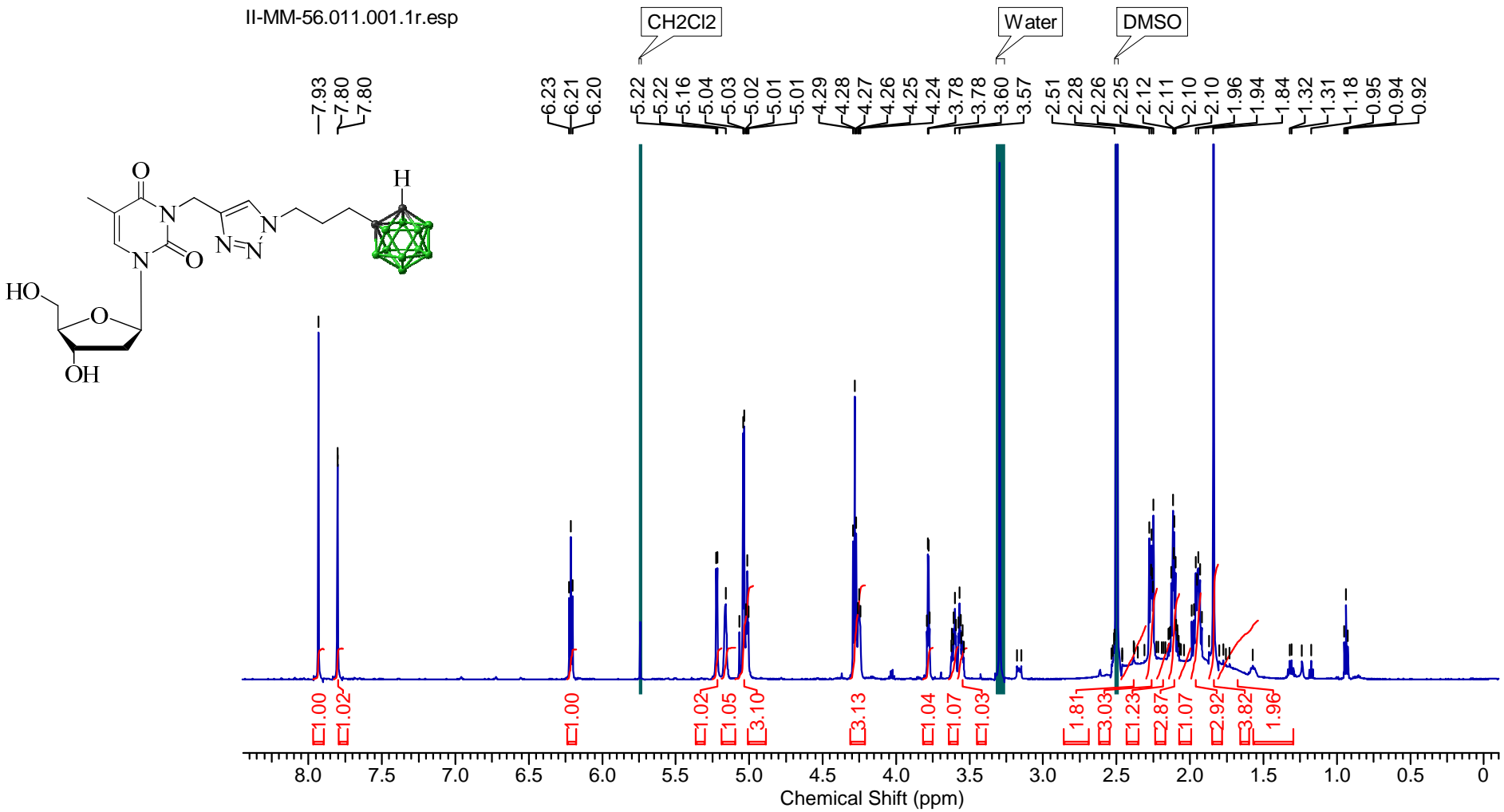


Figure S1. ^1H NMR spectrum of conjugate 20.

II-MM-56.013.001.1r.esp

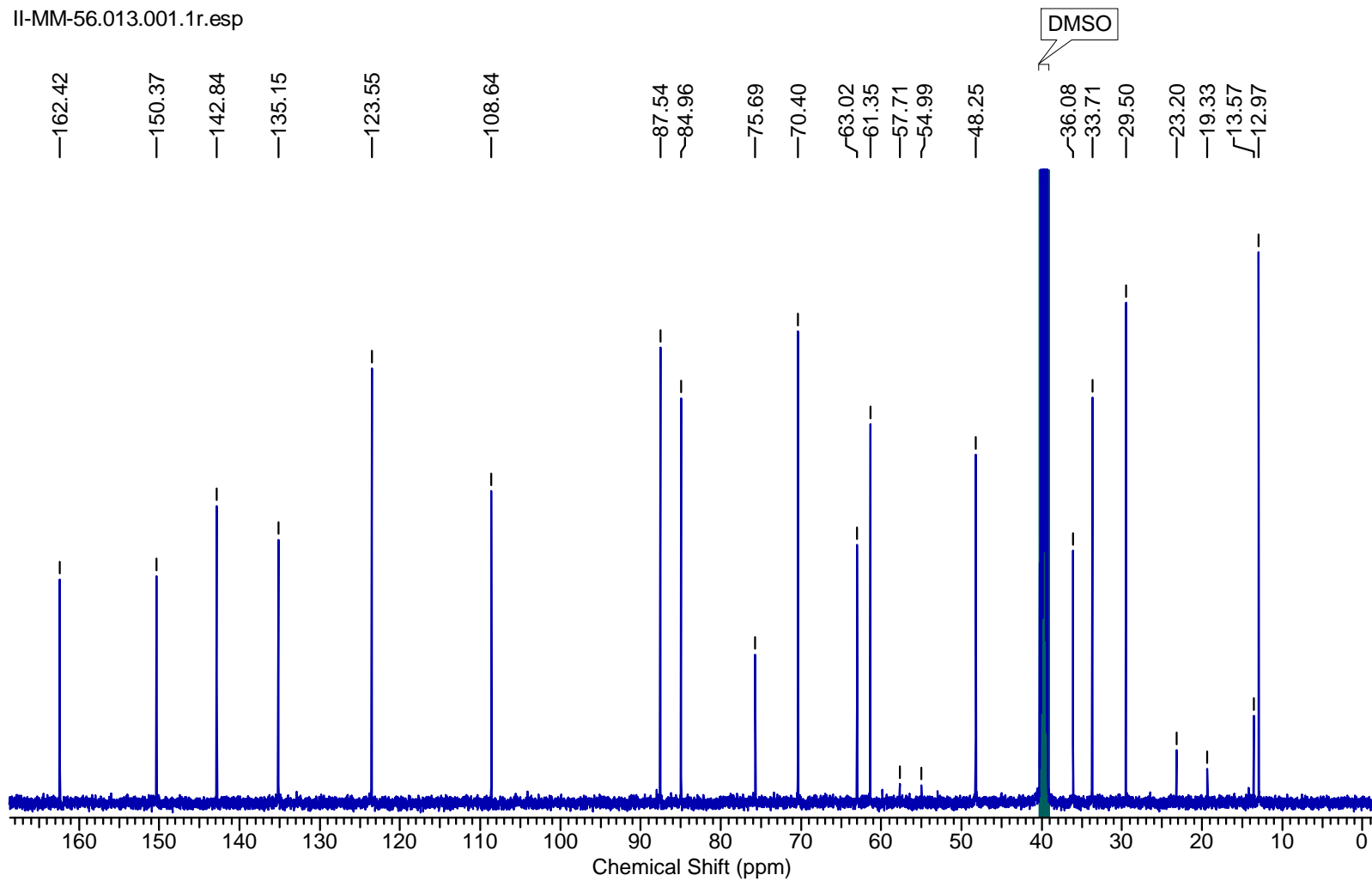


Figure S2. ^{13}C NMR spectrum of conjugate **20**.

II-MM-56.010.001.1r.esp

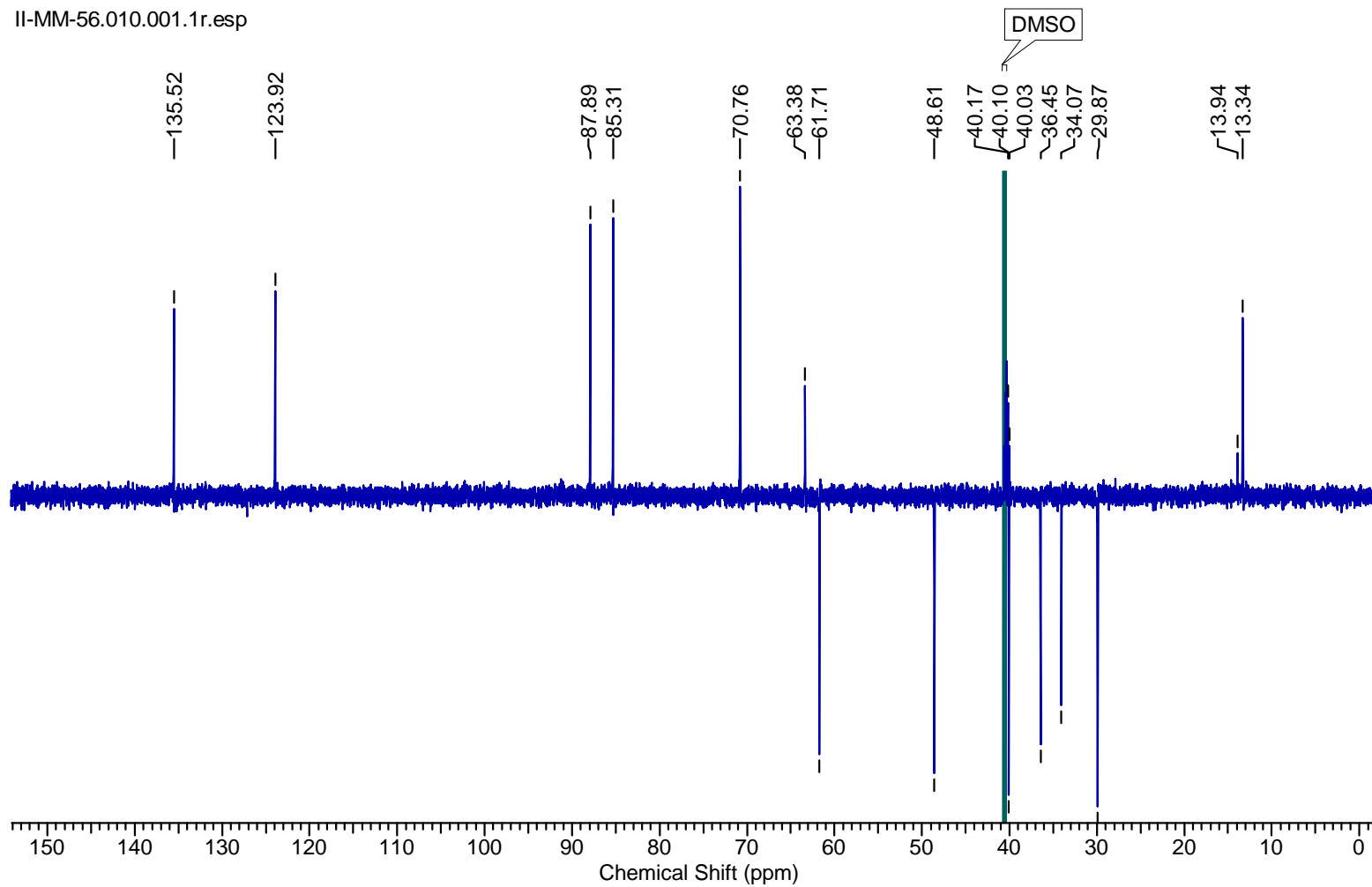


Figure S3. DEPT-135 spectrum of conjugate **20**.

II-MM-56.004.001.1r.esp

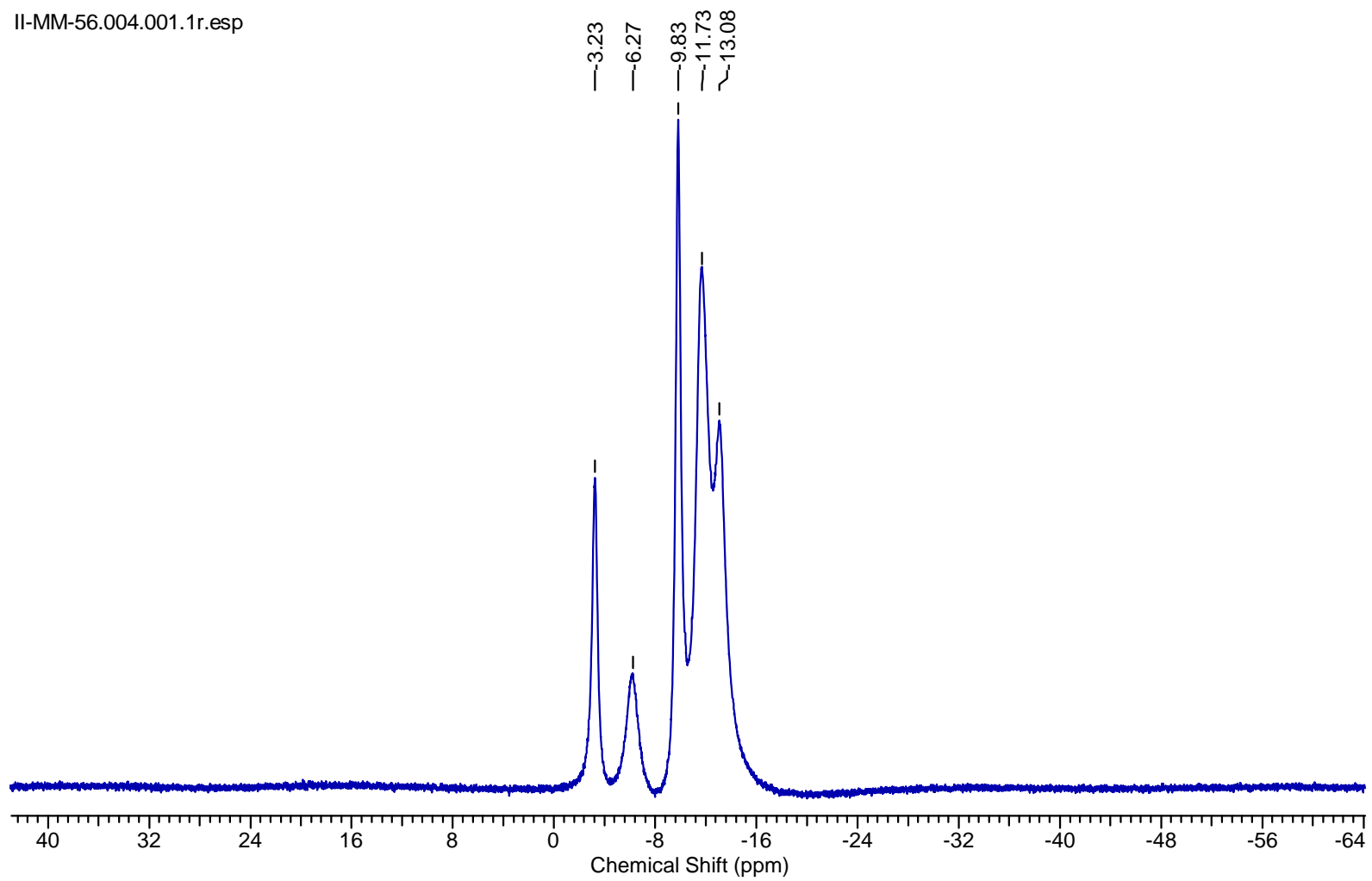


Figure S4. ^{11}B {H BB} NMR spectrum of compound **20**.

II-MM-56.005.001.1r.esp

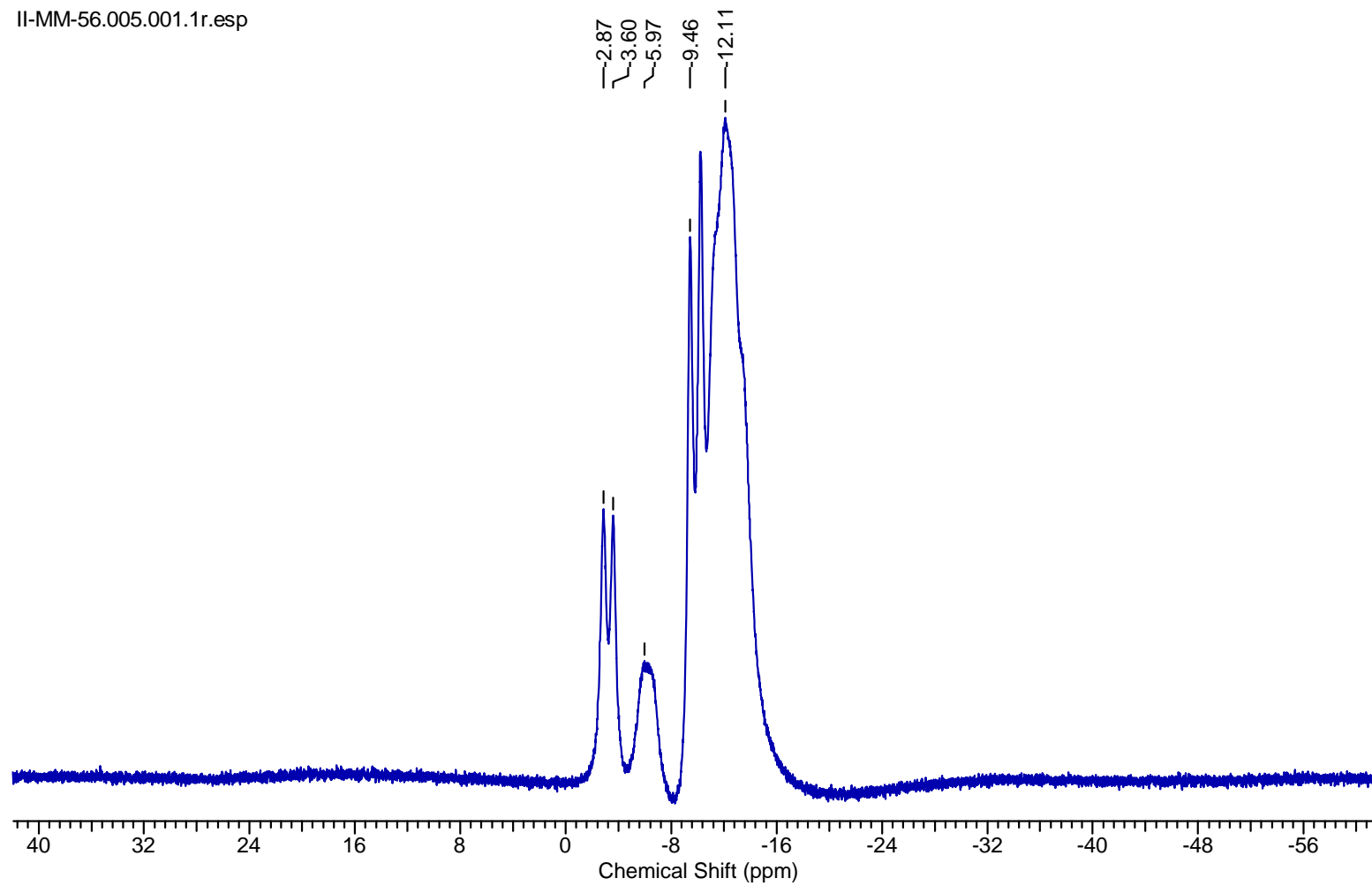


Figure S5. ^{11}B NMR spectrum of compound **20**.

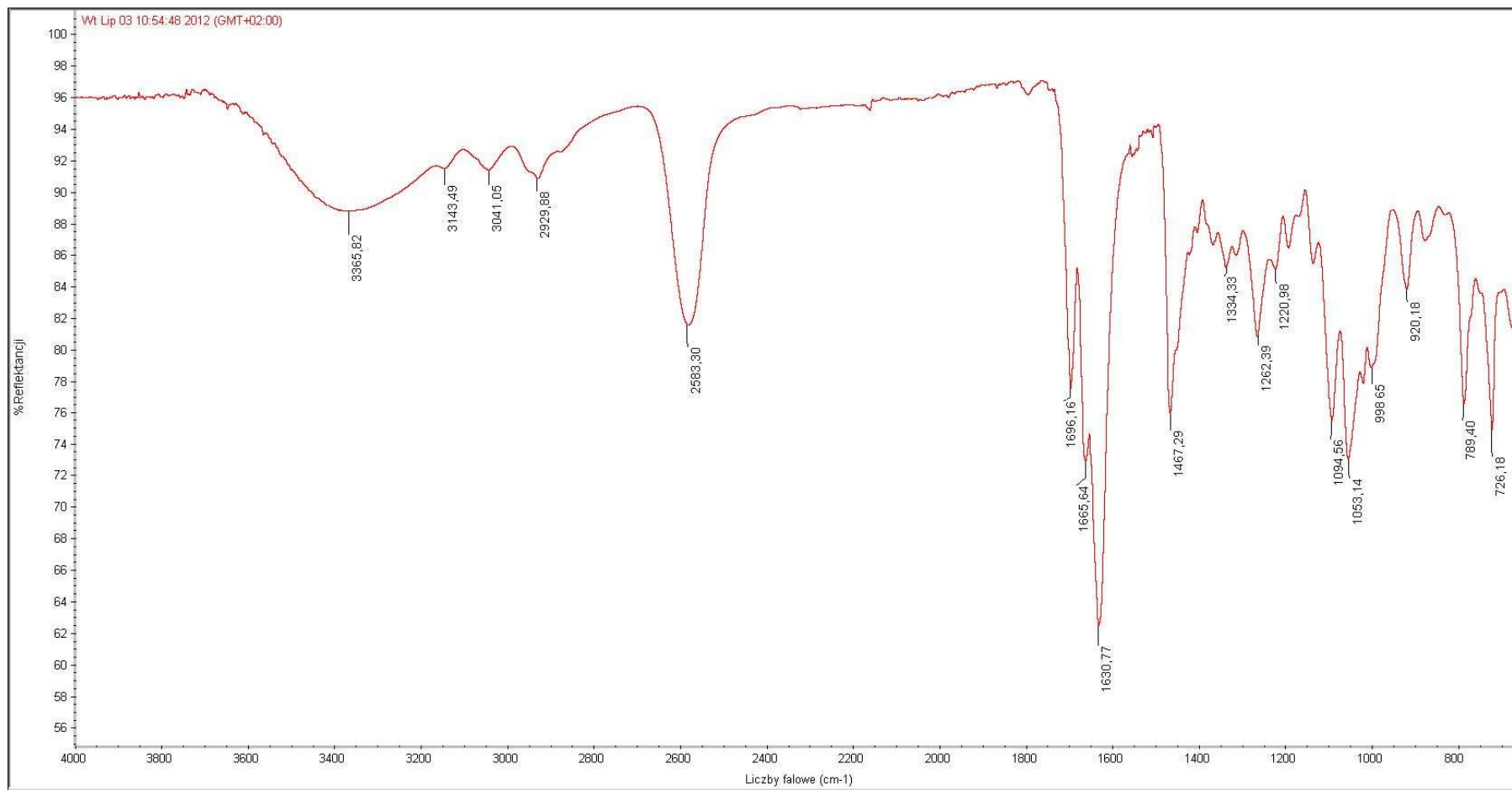
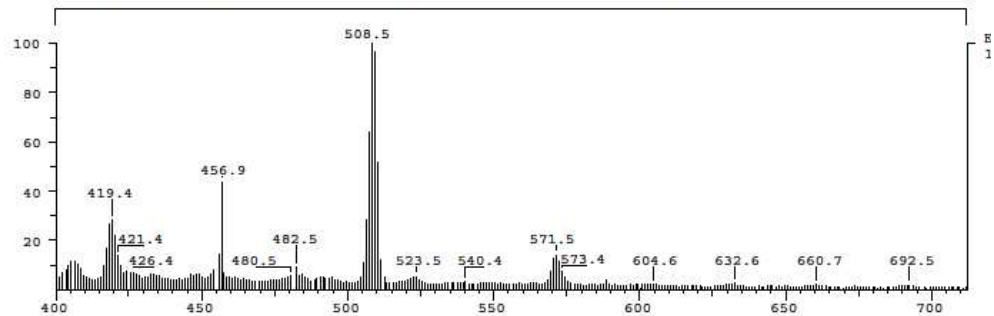
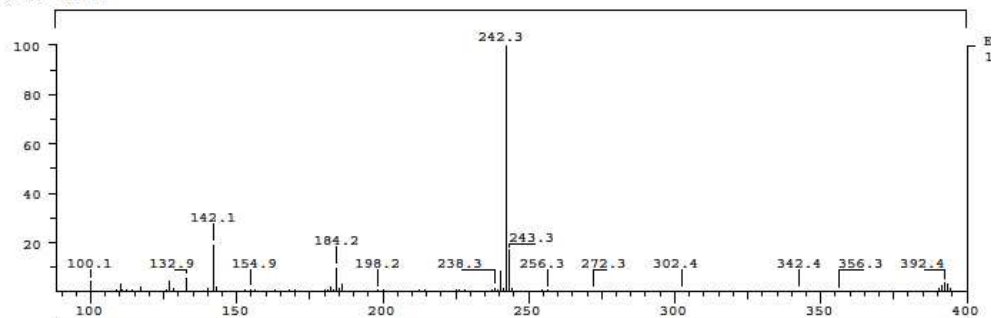


Figure S6. IR spectrum of compound **20**.

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 Comm: LSI, Cs+ 13 keV, gly
 Mode: FAB +VE +LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: es Client: IBM A.Olejniczak Inlet :
 Base: 242.3 Inten : 16414624 Masses: 100 > 1000
 Norm: 242.3 RIC : 45864128 #peaks: 856
 Peak: 1000.00 mmu
 Data: +1>10



SPEC: ax275ibm 04-Apr-12 REG : 00:16.3 #9
 Samp: II-MM-56 Start : 12:41:51 10
 Comm: LSI, Cs+ 13 keV, gly
 Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: es Client: IBM A.Olejniczak Inlet :
 Base: 507.5 Inten : 229403 Masses: 100 > 1000
 Norm: 507.5 RIC : 4362206 #peaks: 879
 Peak: 1000.00 mmu
 Data: +1>10

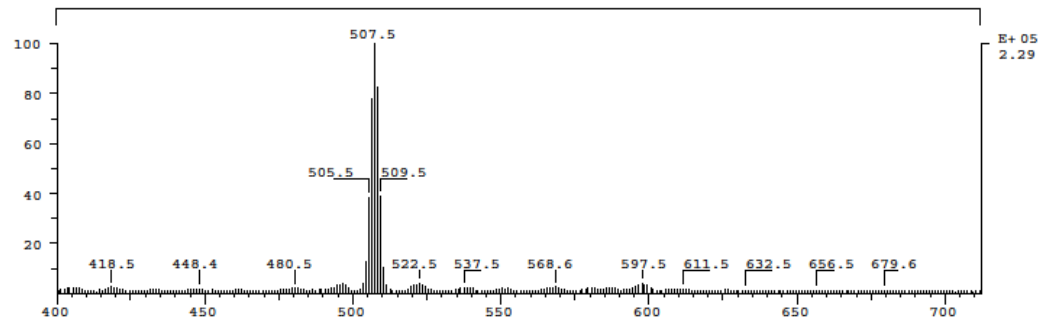
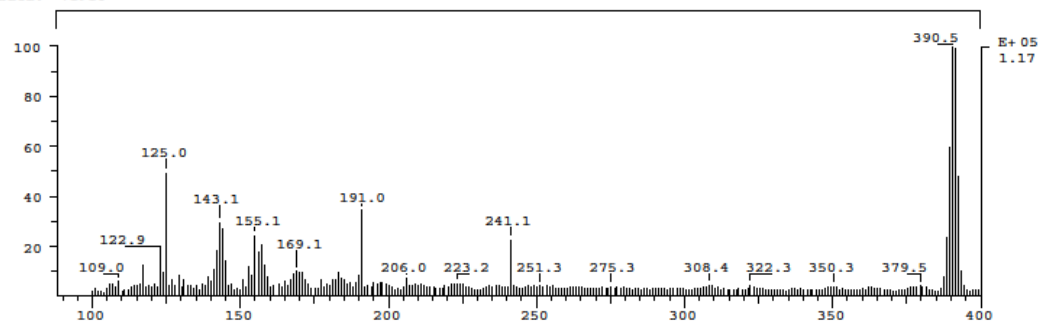


Figure S7. MS-FAB spectra of compound 20.

III-MM-43.010.001.1r.esp

Water

DMSO

7.94
7.59
7.59
7.39
7.38
7.31
7.29
7.26
7.25
6.90
6.90
6.88
6.88
6.27
6.26
6.25
5.74
5.32
5.31
5.15
5.05
5.04
4.34
4.34
4.33
4.29
4.28
4.27
3.91
3.91
3.74
3.23
3.22
3.21
3.21
2.28
2.27
2.26
2.26
2.25
2.25
1.96
1.95
1.95
1.93
1.50
1.50

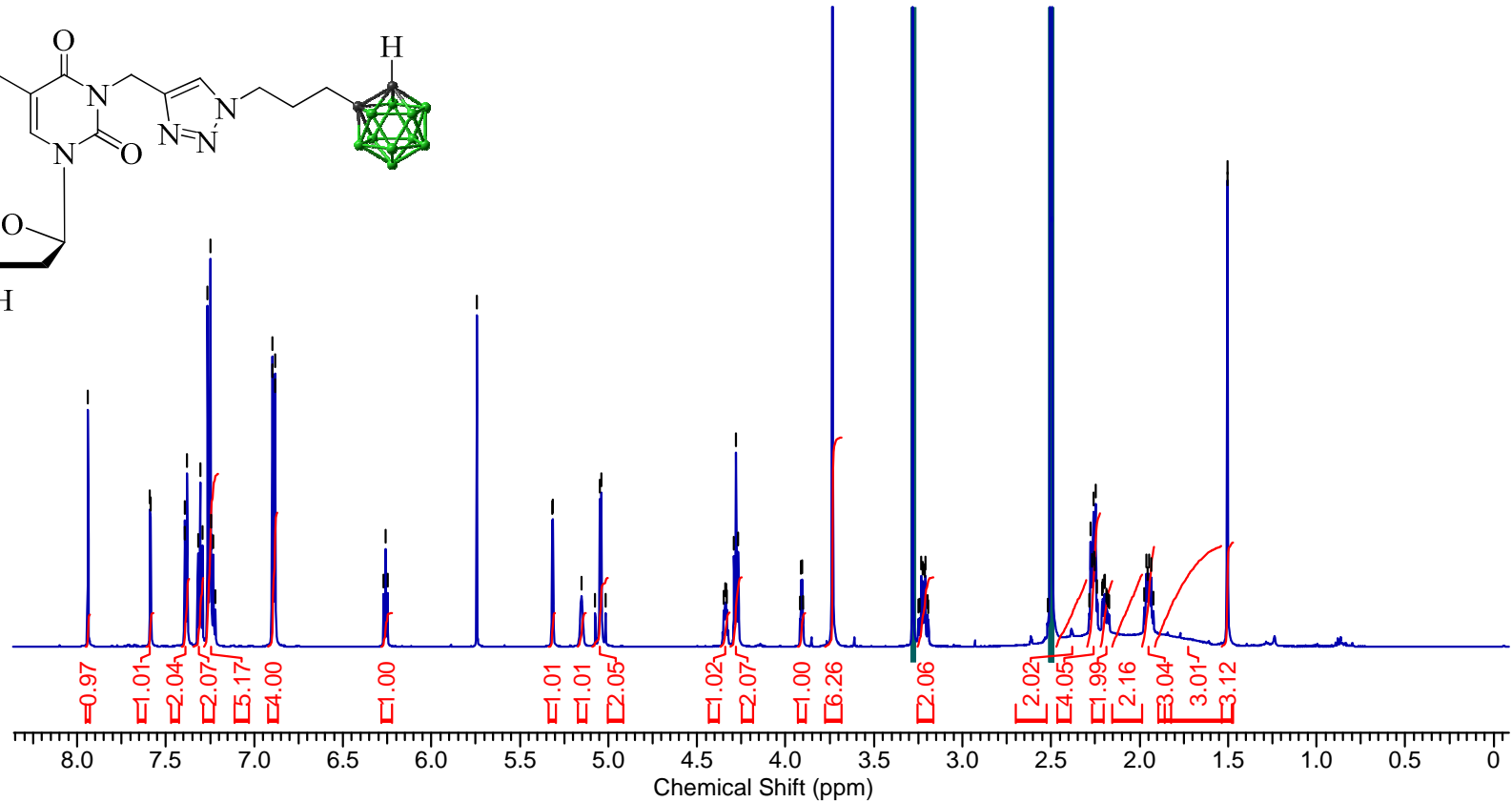
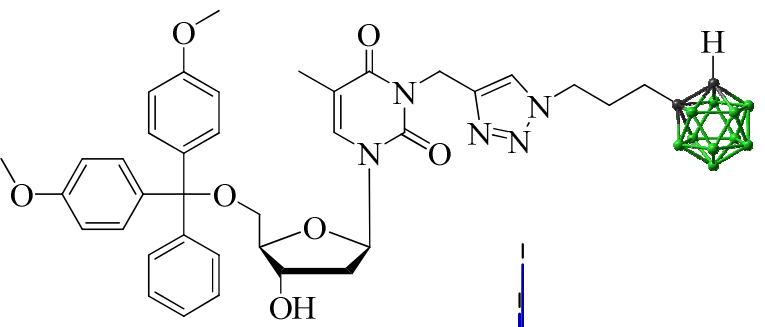


Figure S8. ¹H NMR spectrum of compound 21.

III-MM-43.020.001.1r.esp

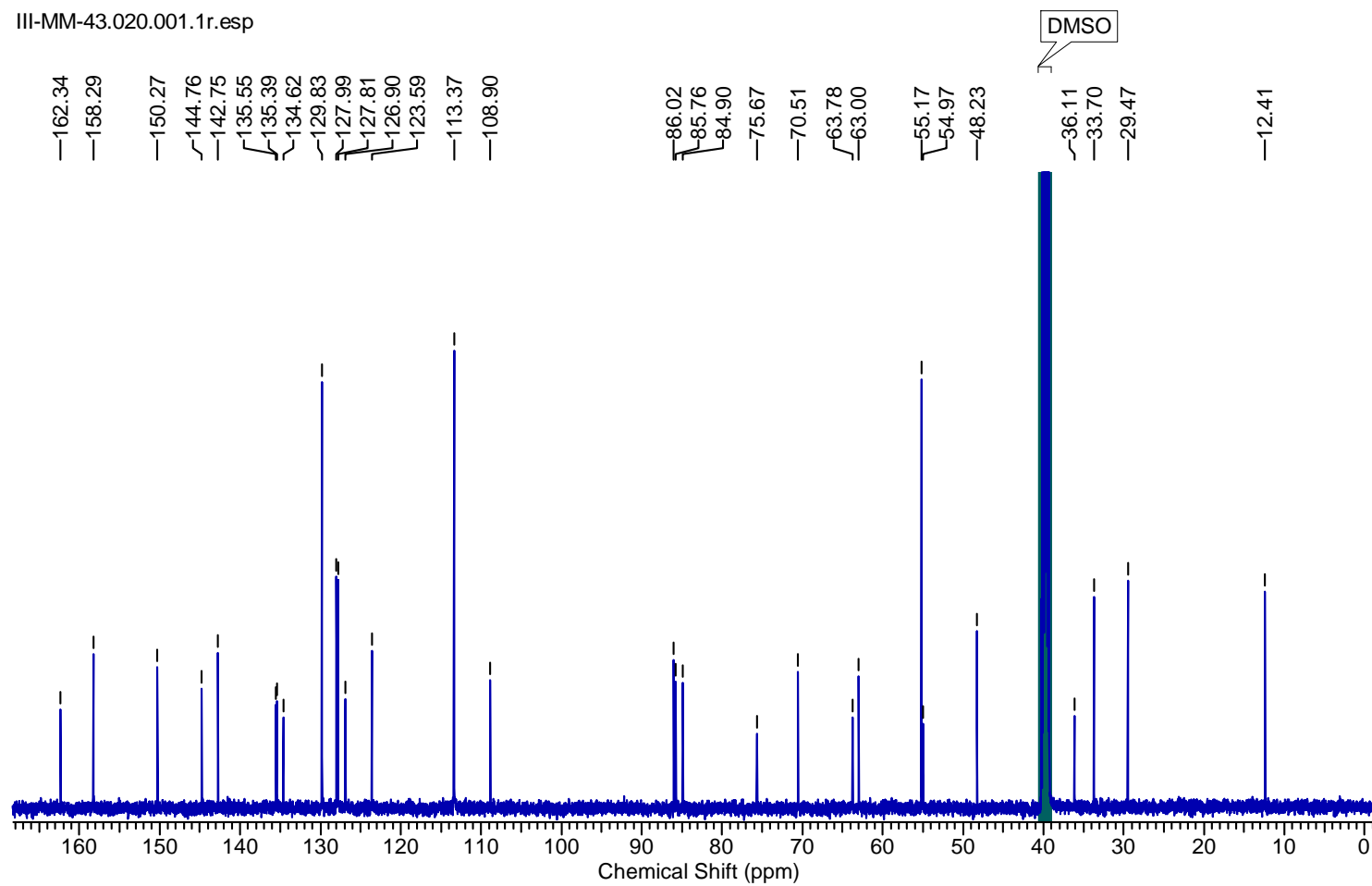


Figure S9. ^{13}C NMR spectrum of compound **21**.

III-MM-43.021.001.1r.esp

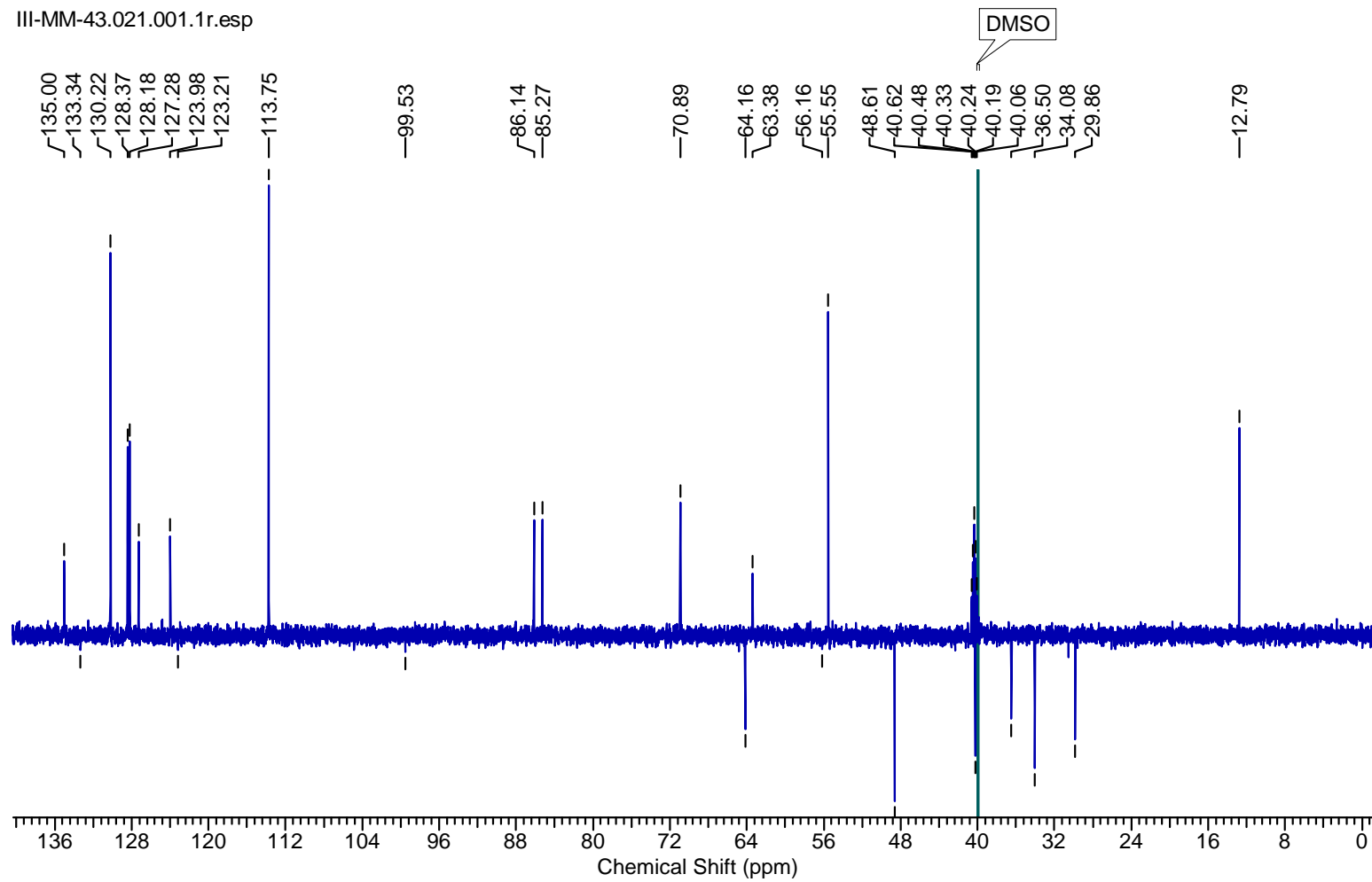


Figure S10. DEPT-135 spectrum of compound **21**.

III-MM-43.003.001.1r.esp

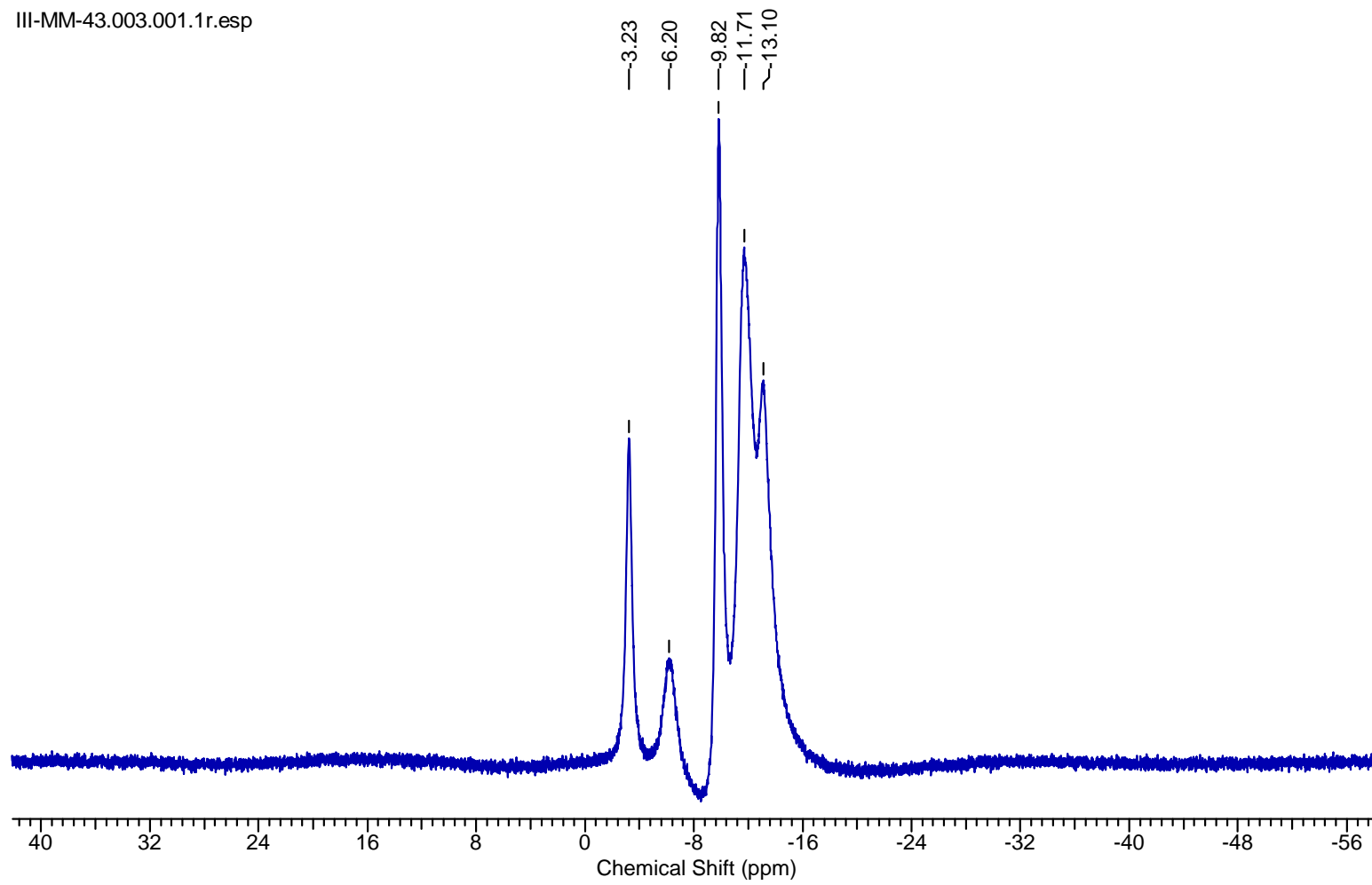


Figure S11. ^{11}B {H BB} NMR spectrum of compound **21**.

III-MM-43.004.001.1r.esp

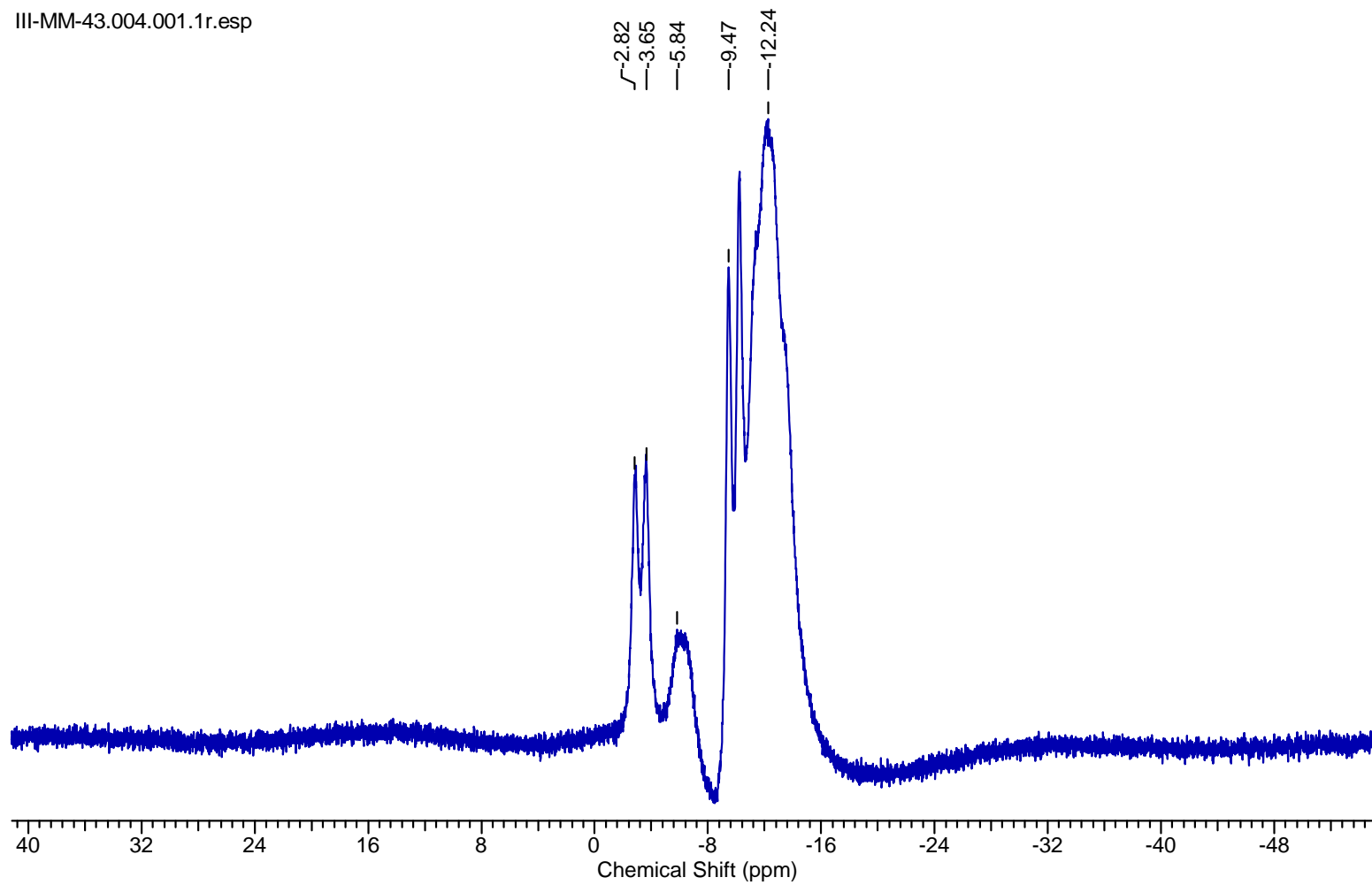


Figure S12. ^{11}B NMR spectrum of compound **21**.

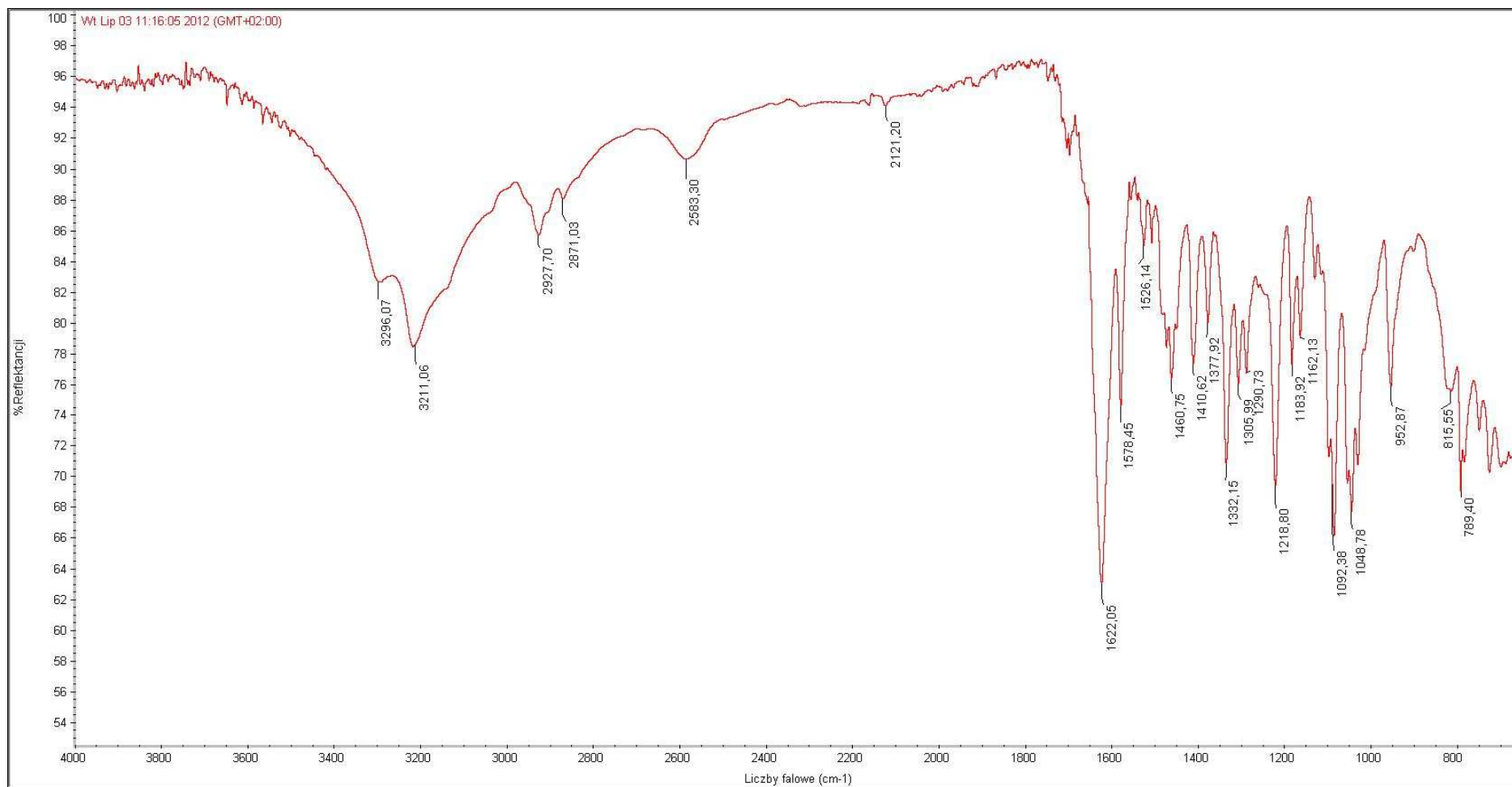


Figure S13. IR spectrum of compound **21**.

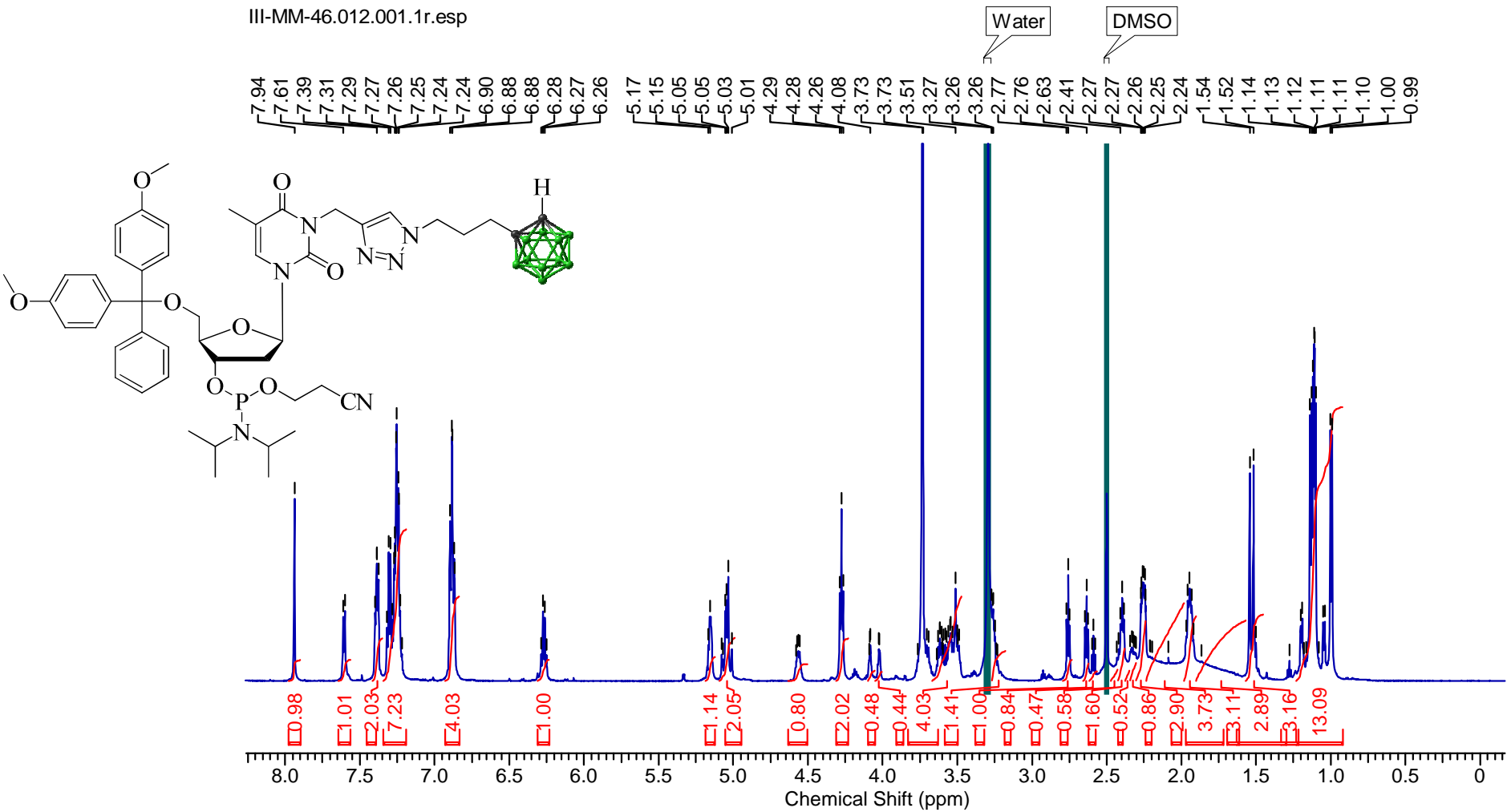


Figure S15. ^1H NMR spectrum of compound 29.

III-MM-46.010.001.1r.esp

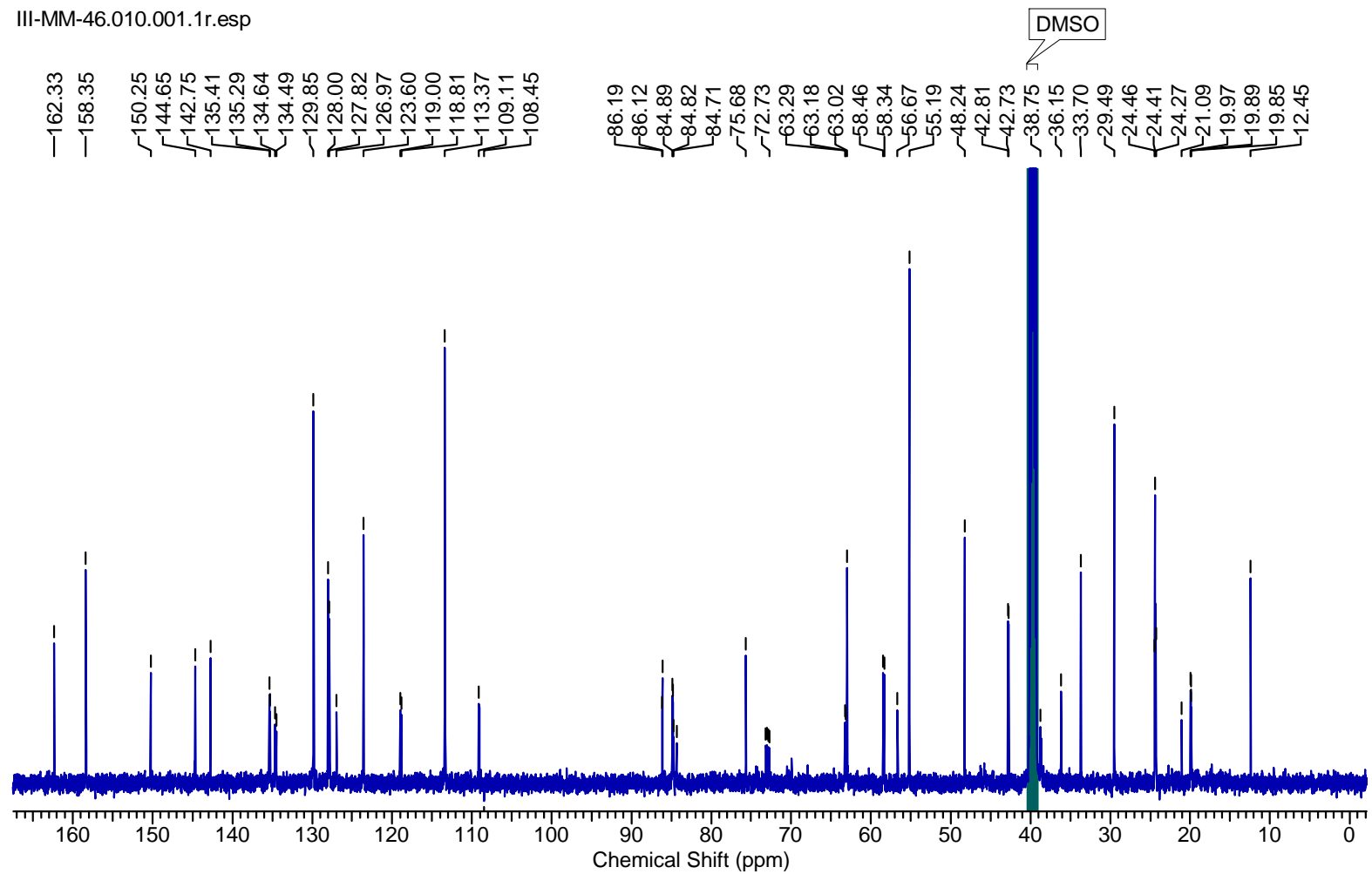


Figure S16. ^{13}C NMR spectrum of compound **29**.

III-MM-46.011.001.1r.esp

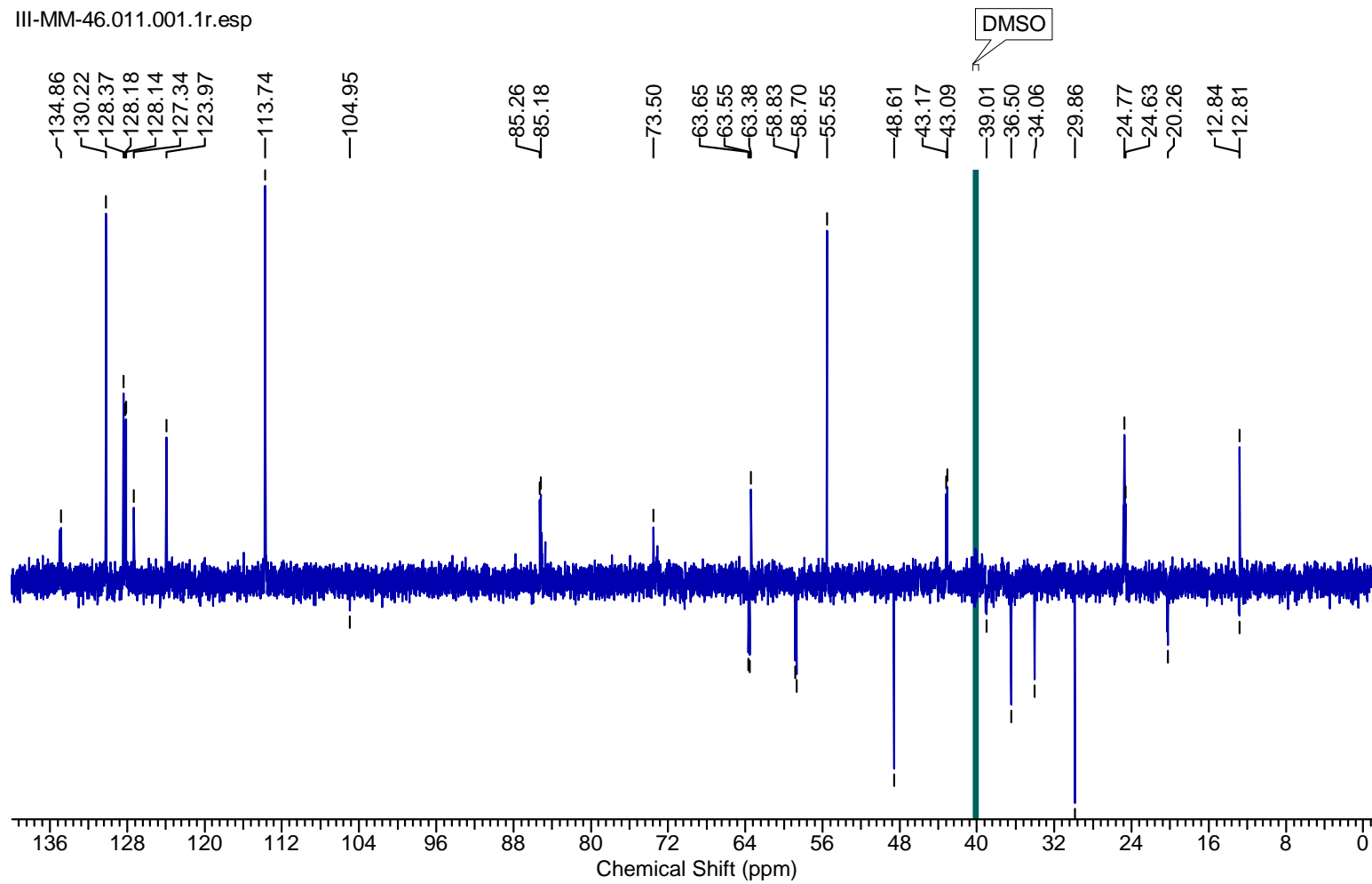


Figure S17. DEPT-135 spectrum of compound **29**.

III-MM-46.003.001.1r.esp

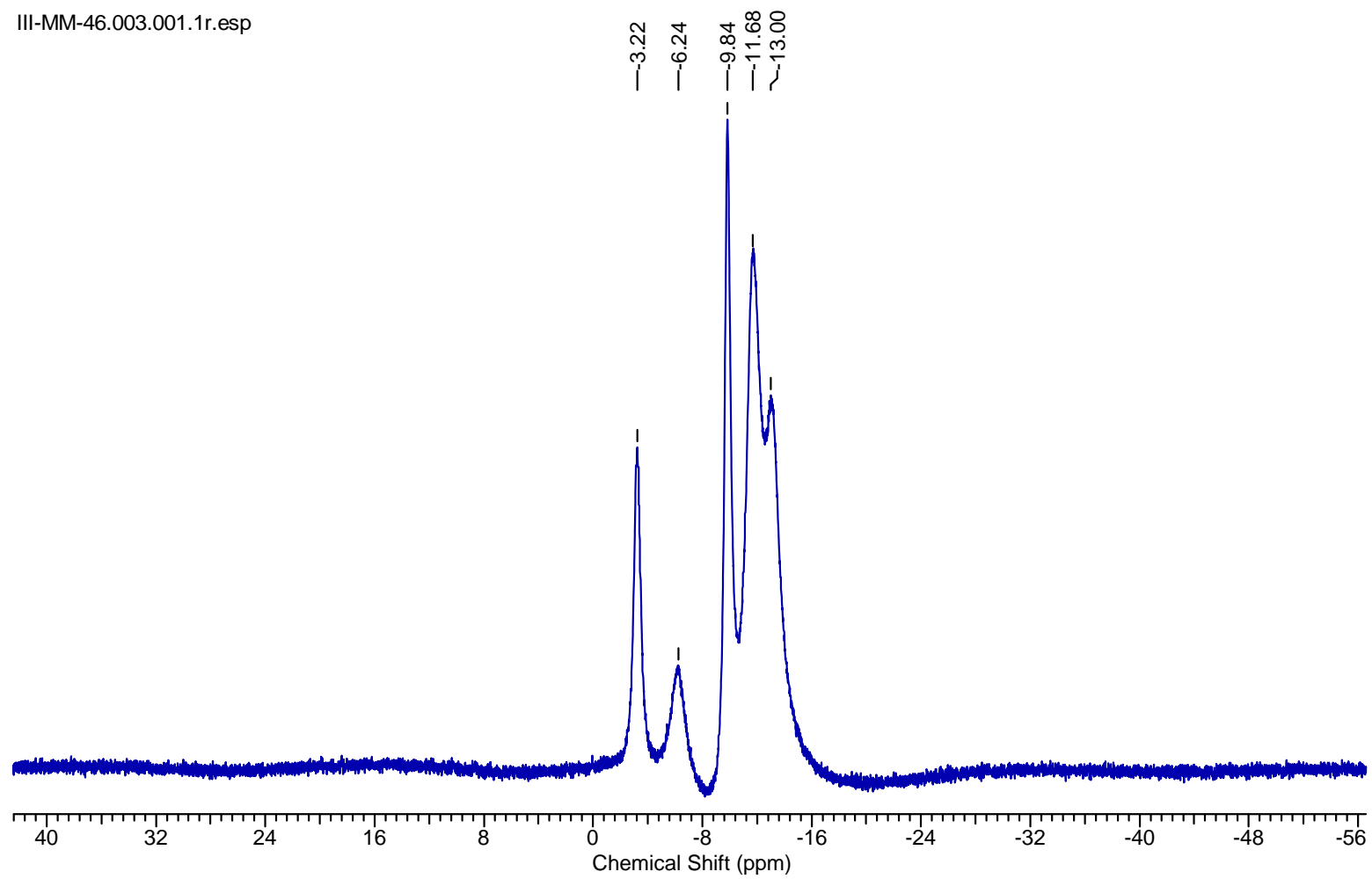


Figure S18. ^{11}B {H BB} NMR spectrum of compound **29**.

III-MM-46.004.001.1r.esp

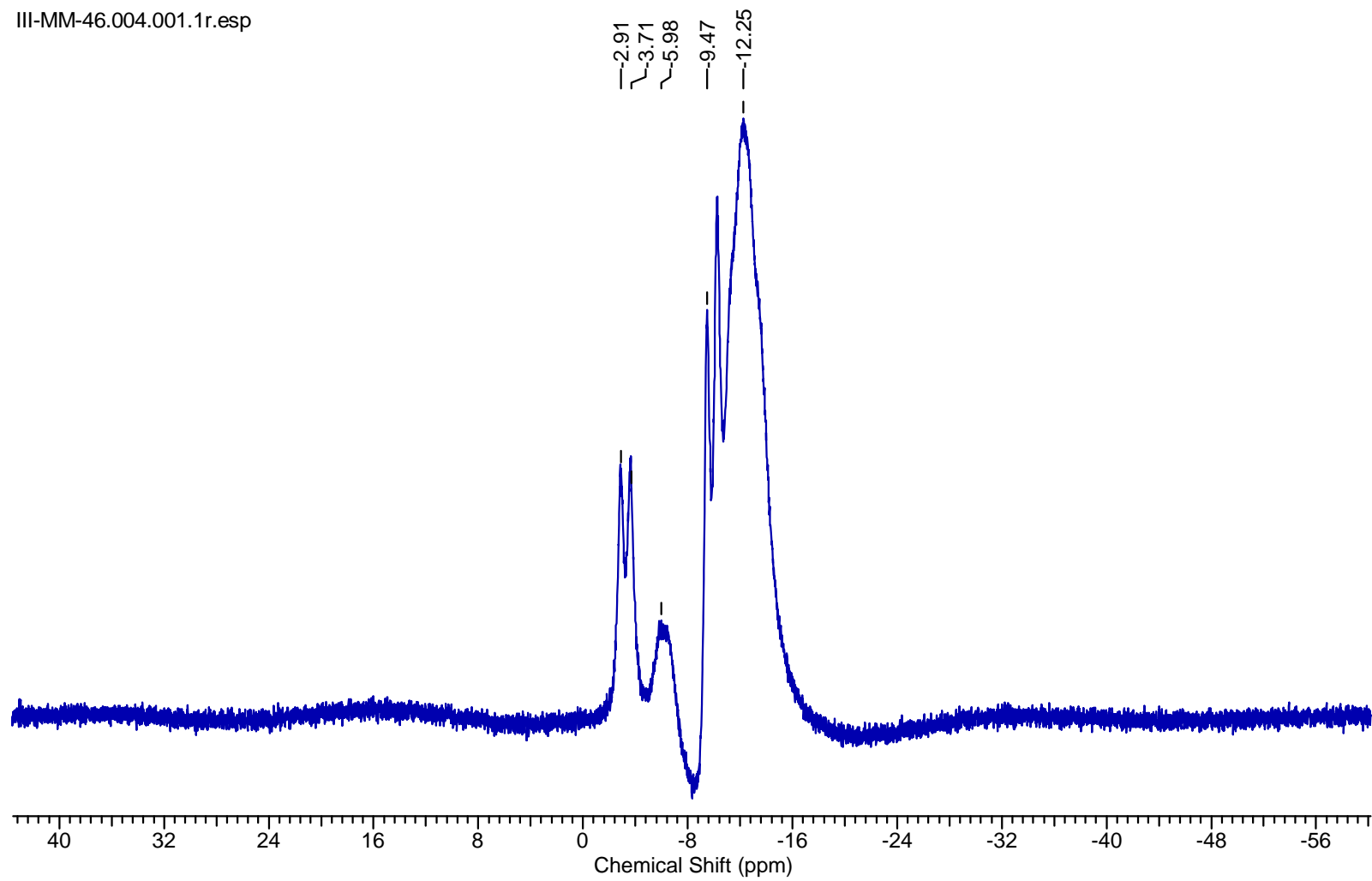


Figure S19. ^{11}B NMR spectrum of compound **29**.

III-MM-46.005.001.1r.esp

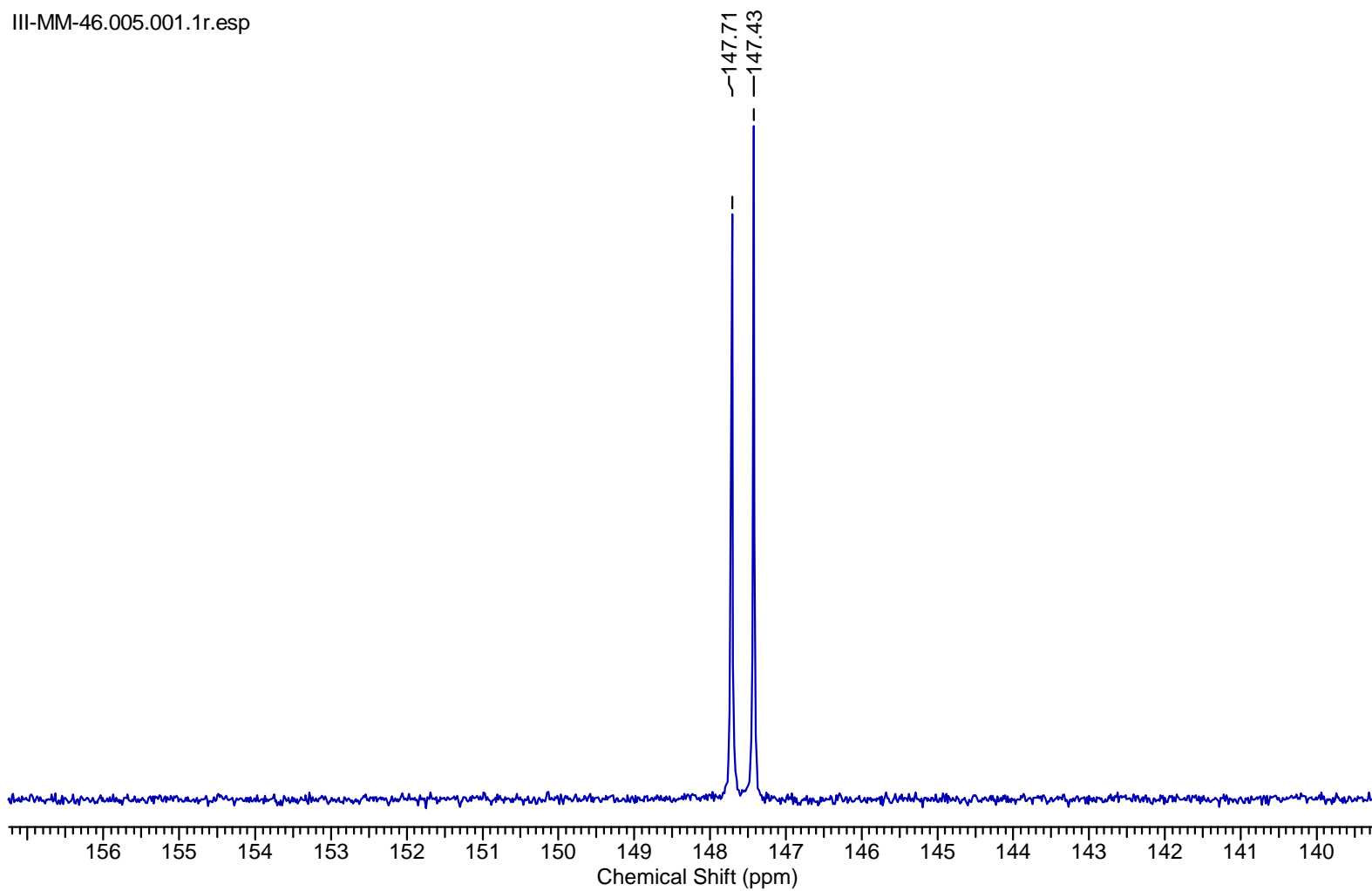


Figure S20. ^{31}P NMR spectrum of compound **29**.

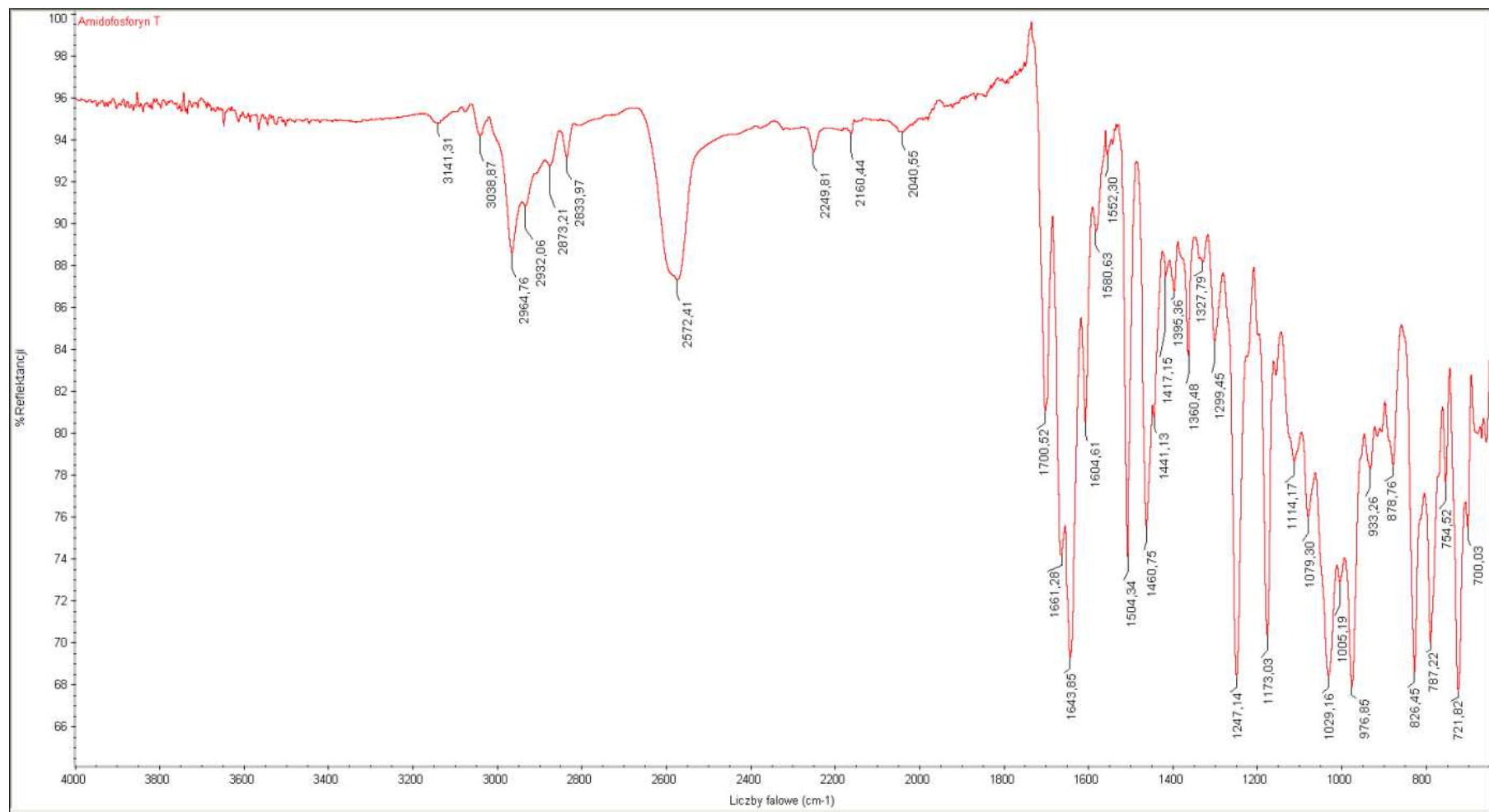
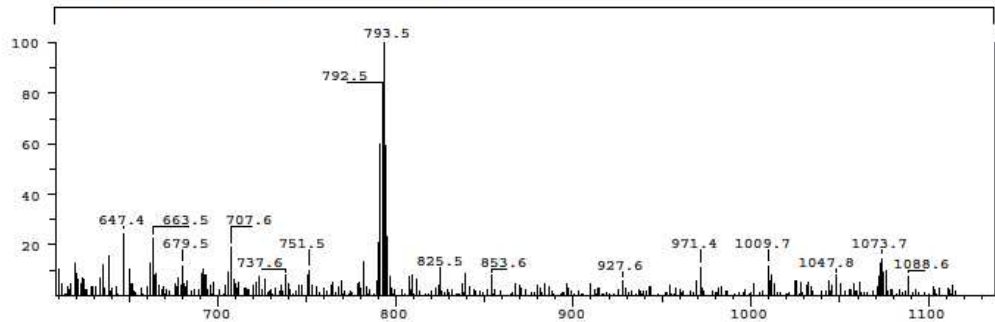
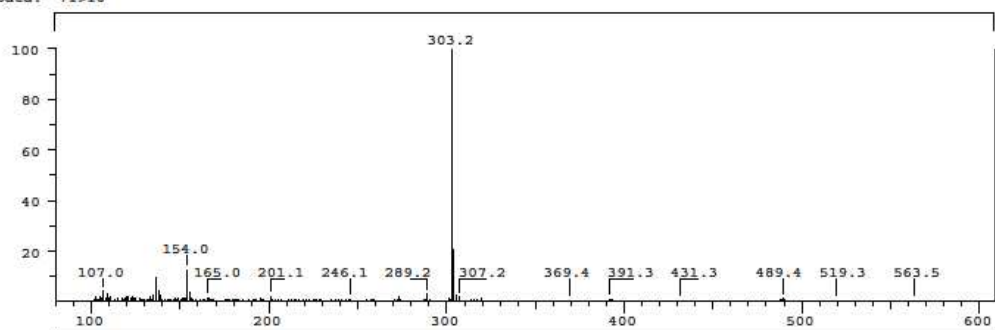


Figure S21. IR spectrum of compound 29.

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 Comm: LSI, Cs+ 13 keV, nba
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 Oper: ed Client: IBM A.Olejniczak Inlet :
 Base: 303.2 Inten : 2381322 Masses: 100 > 1117
 Norm: 303.2 RIC : 8557821 #peaks: 789
 Peak: 1000.00 mmu
 Data: +1>10



SPEC: ax745ibm b 12-Jul-12 REG : 00:16.8 #9
 Samp: III-MM-46 Start : 09:33:45 10
 Comm: LSI, Cs+ 13 keV, nba
 Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ed Client: IBM A.Olejniczak Inlet :
 Base: 152.9 Inten : 220419 Masses: 100 > 1117
 Norm: 152.9 RIC : 3129984 #peaks: 672
 Peak: 1000.00 mmu
 Data: +1>10

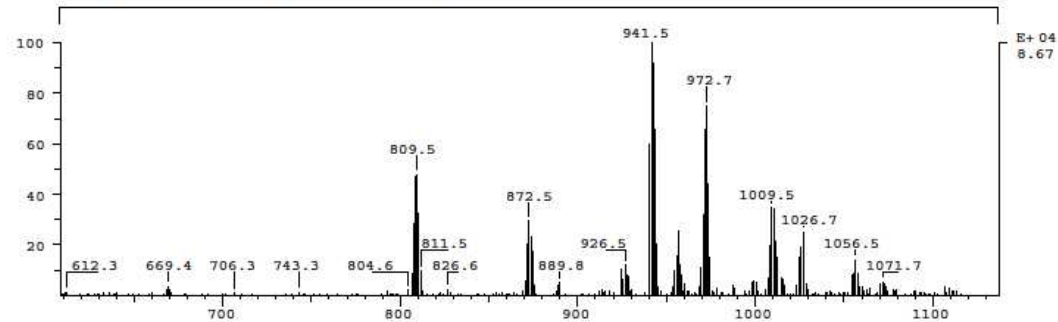
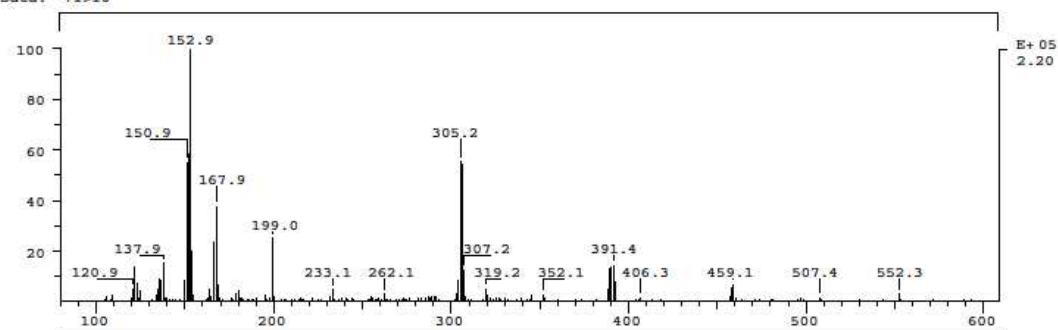


Figure S22. MS-FAB spectra of compound 29.

II-MM-49.010.001.1r.esp

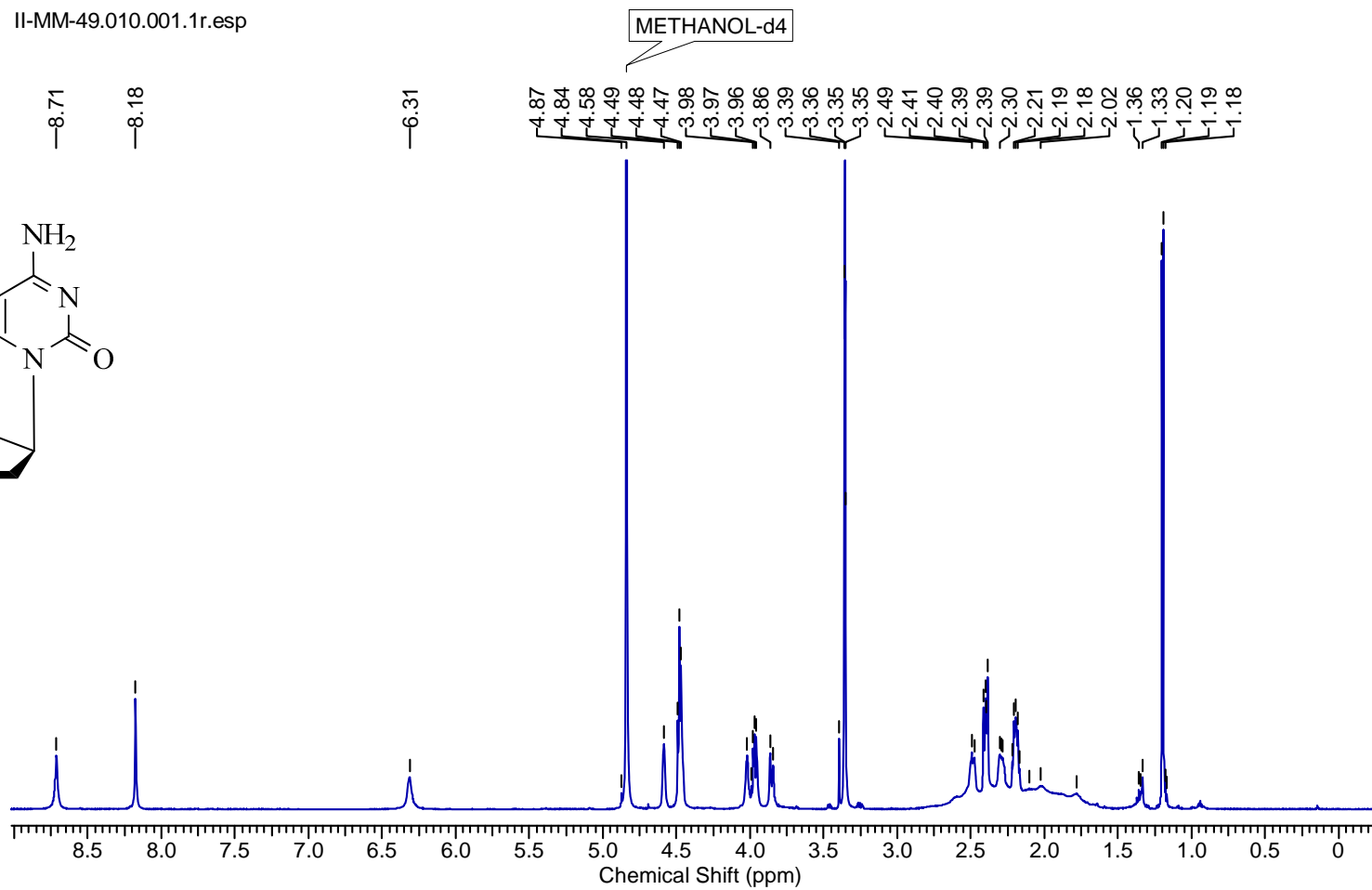
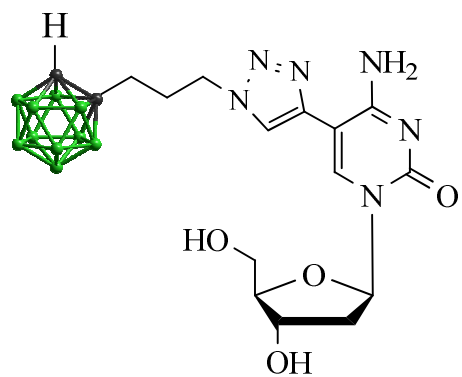


Figure S23. ^1H NMR spectrum of compound **22**.

II-MM-49.013.001.1r.esp

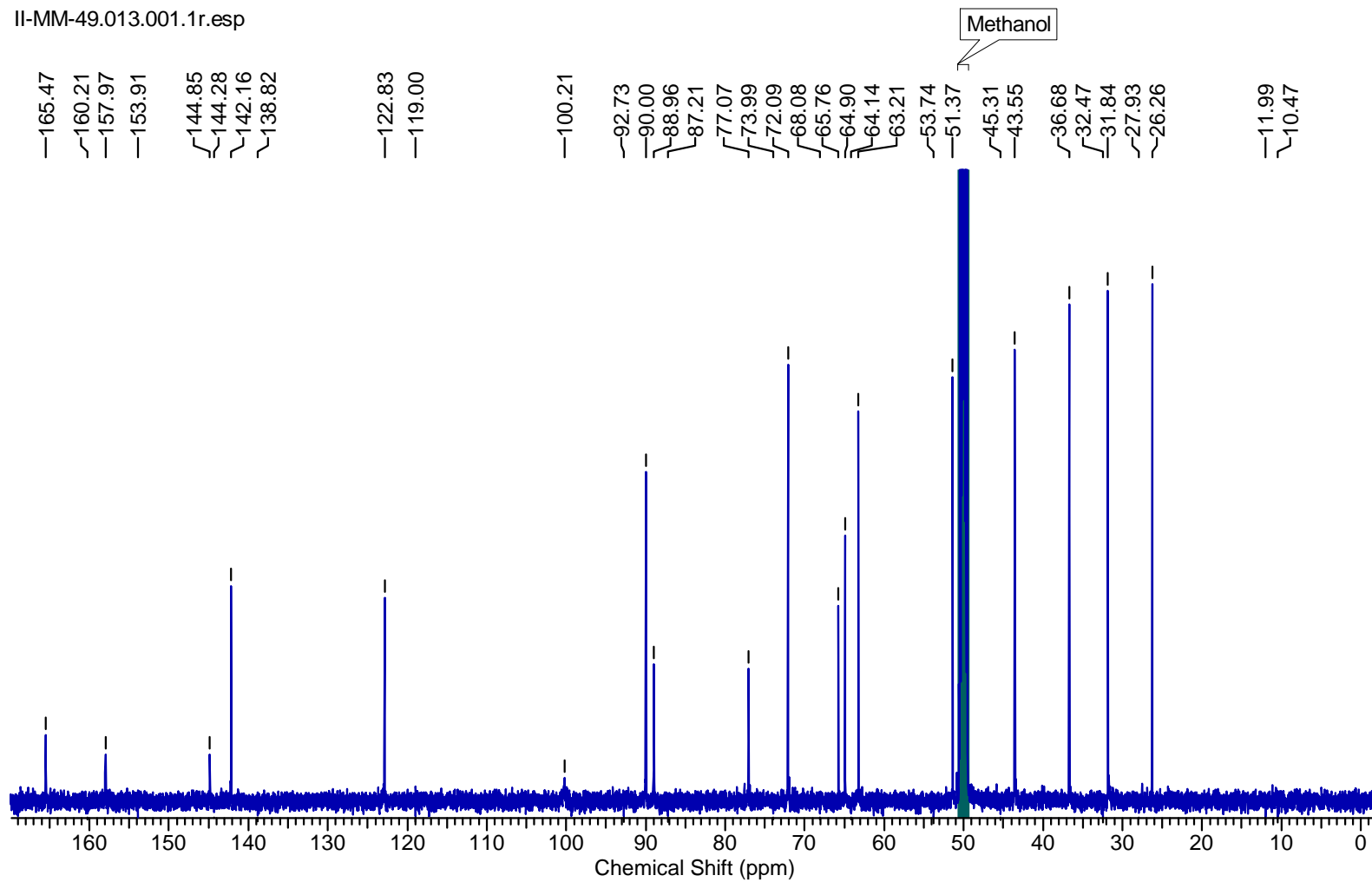


Figure S24. ^{13}C NMR spectrum of compound 22.

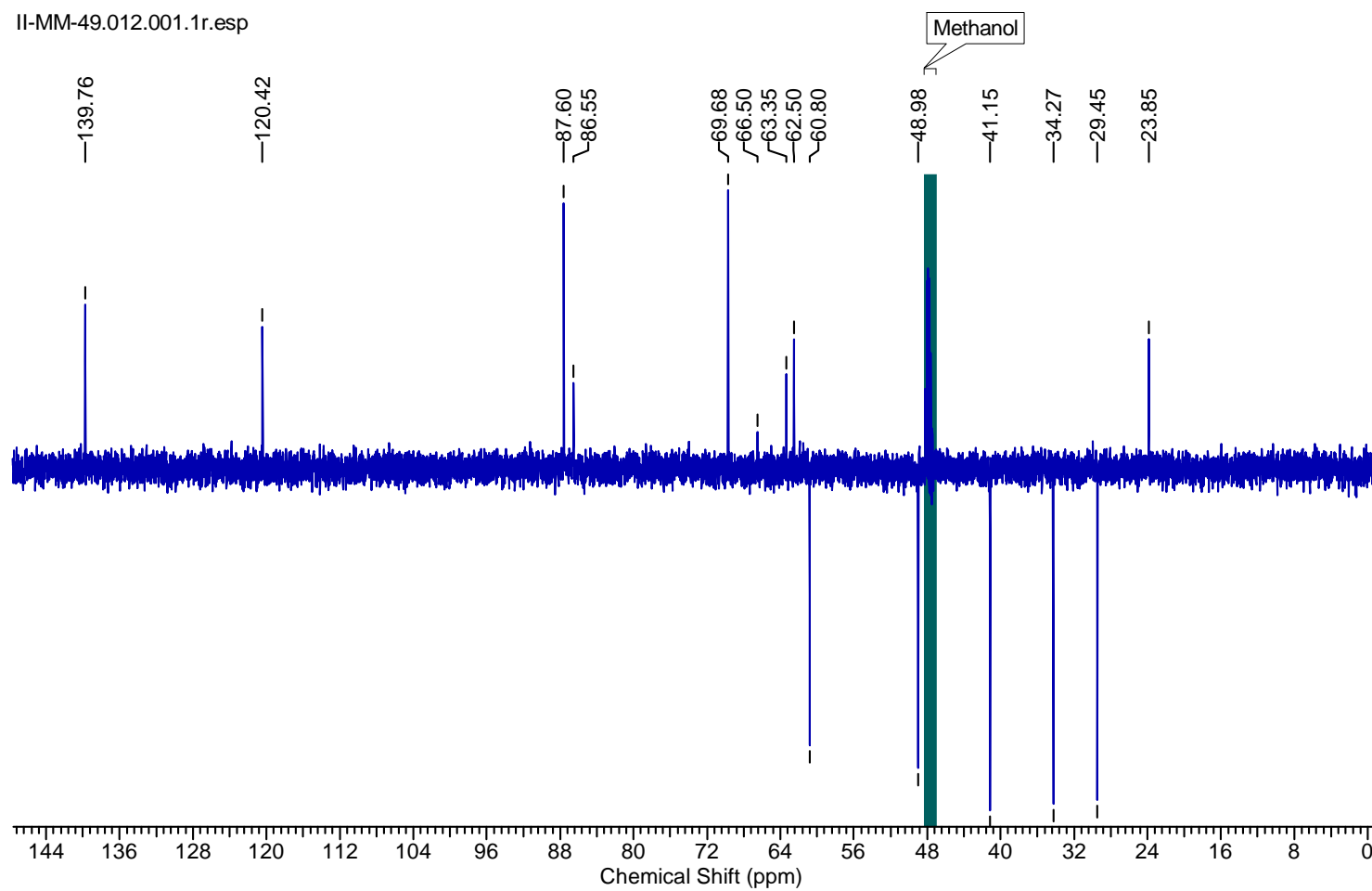


Figure S25. DEPT-135 spectrum of compound **22**.

II-MM-49.005.001.1r.esp

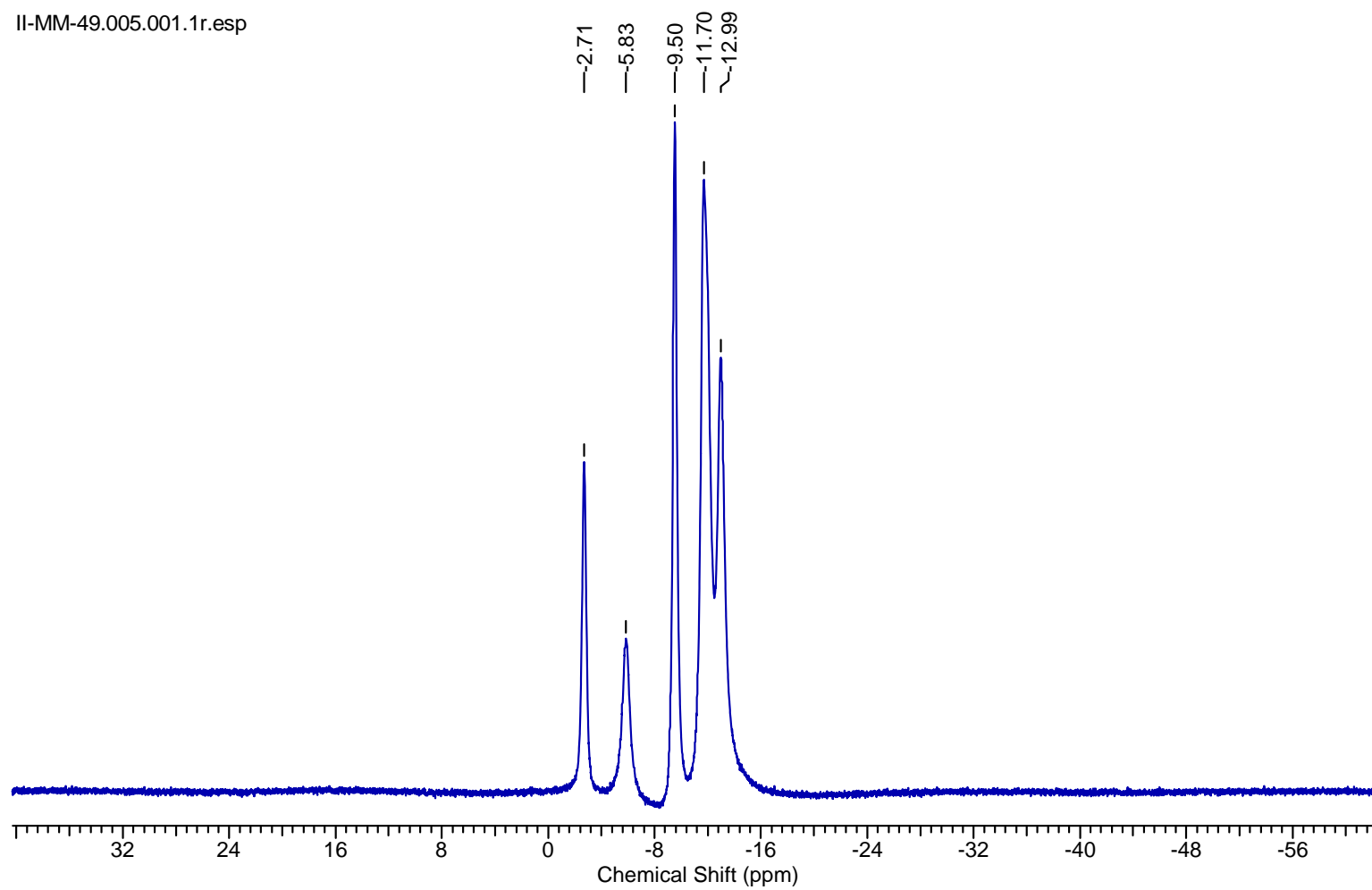


Figure S26. ^{11}B {H BB} NMR spectrum of compound **22**.

II-MM-49.006.001.1r.esp

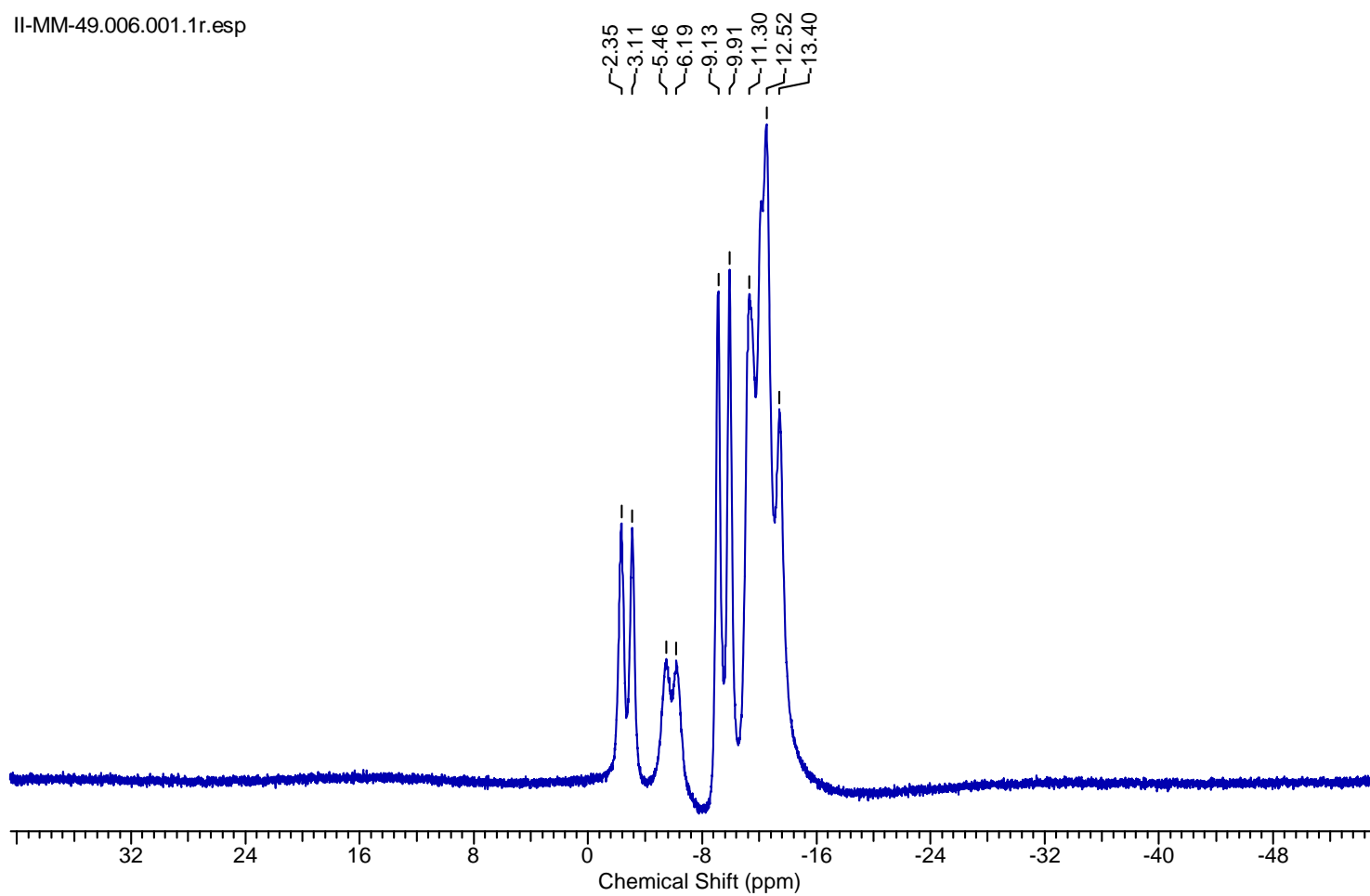


Figure S27. ^{11}B NMR spectrum of compound **22**.

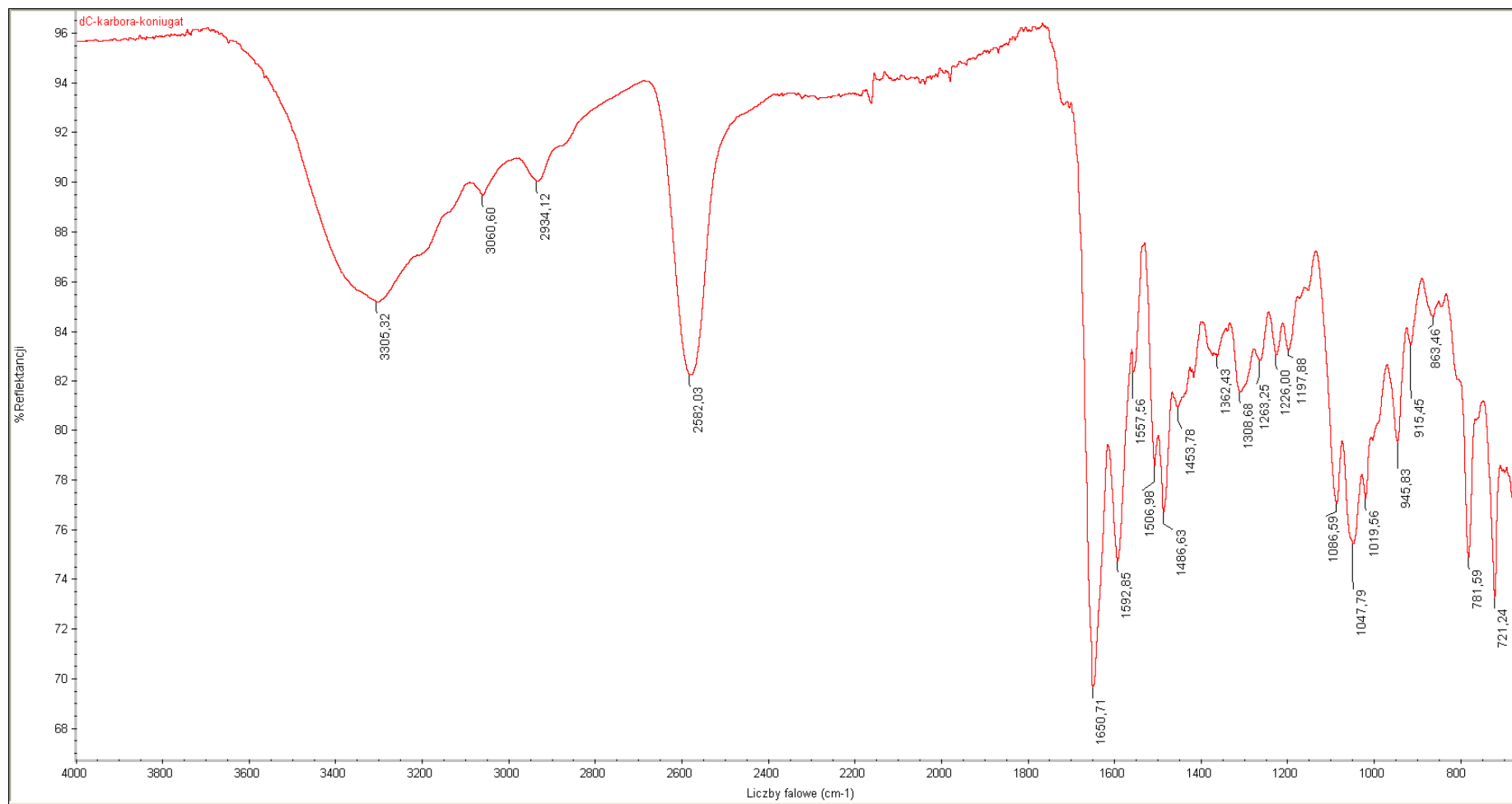
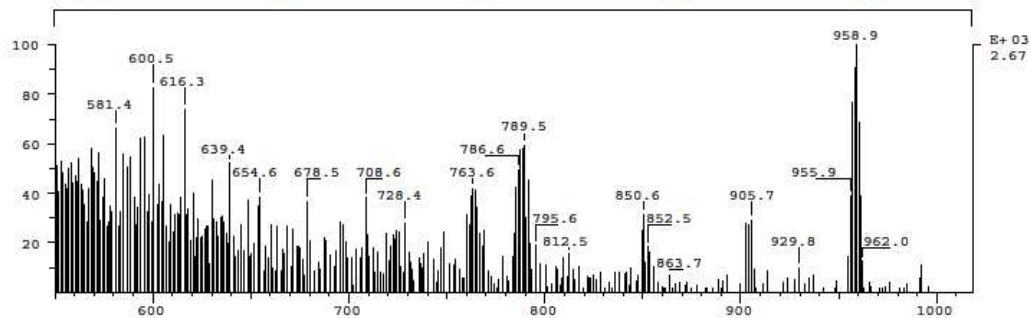
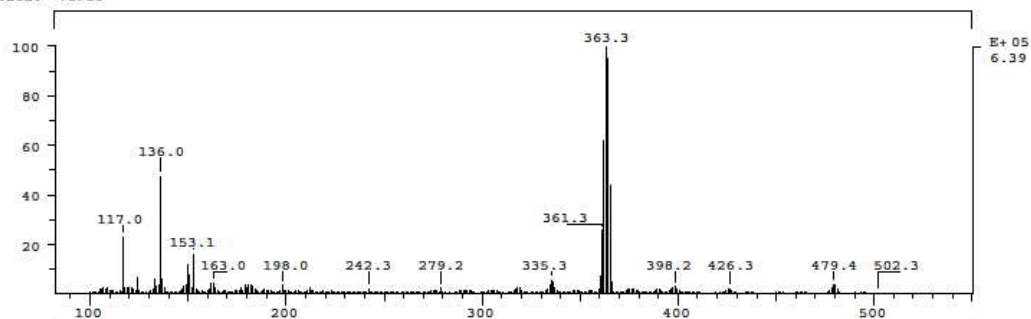


Figure S28. IR spectrum of compound **22**.

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 Oper: es Client: IBM A.Olejniczak Inlet :
 Base: 363.3 InLen : 638819 Masses: 100 > 1000
 Norm: 363.3 RIC : 5927654 #peaks: 745
 Peak: 1000.00 mmu
 Data: +1>10



SPEC: ax2221bm_b 28-Mar-12 REG : 00:16.4 #9
 Samp: 11-MM-49 Start : 11:53:31 10
 Comm: LSI, Cs+ 13 keV, gly
 Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: es Client: IBM A.Olejniczak Inlet :
 Base: 478.4 Inten : 465097 Masses: 100 > 1000
 Norm: 478.4 RIC : 14533607 #peaks: 900
 Peak: 1000.00 mmu
 Data: +1>10

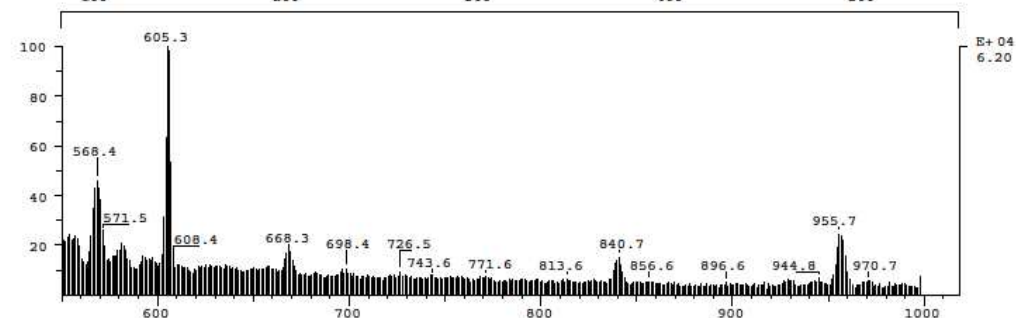
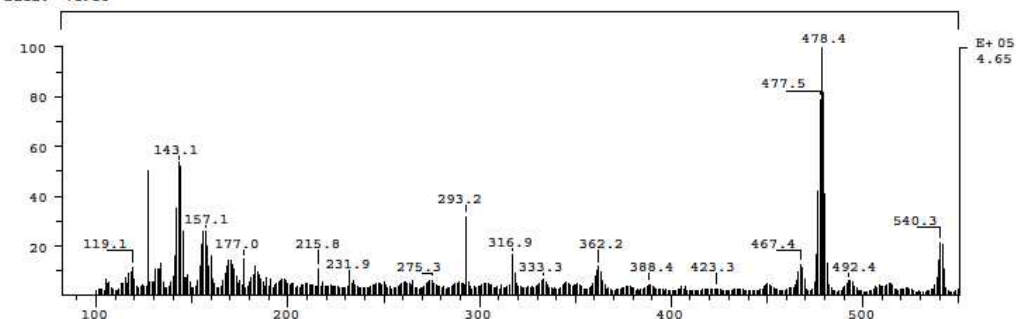


Figure S29. MS-FAB spectra of compound 22.

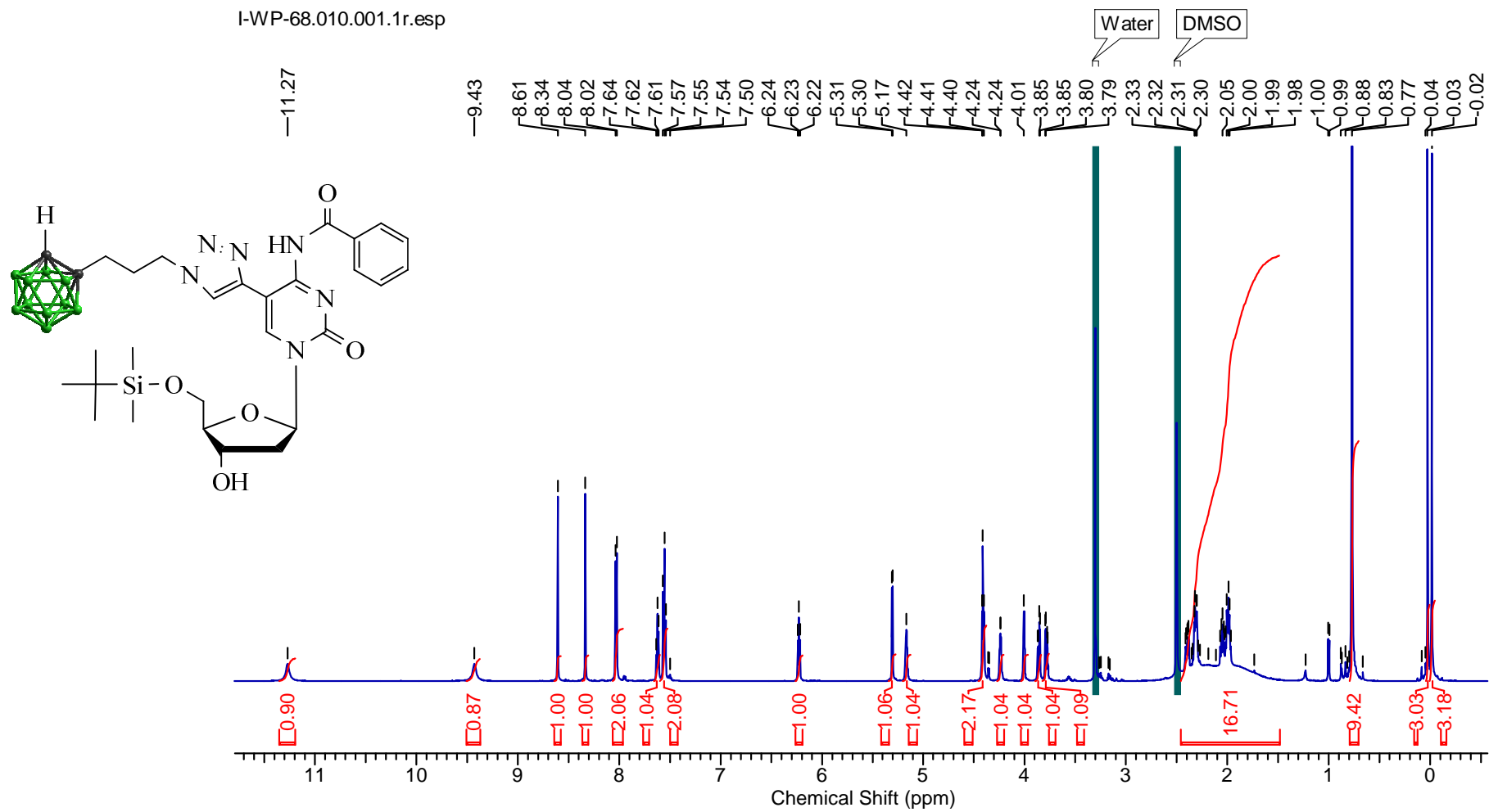


Figure S30. ^1H NMR spectrum of compound 23.

I-WP-68.012.001.1r.esp

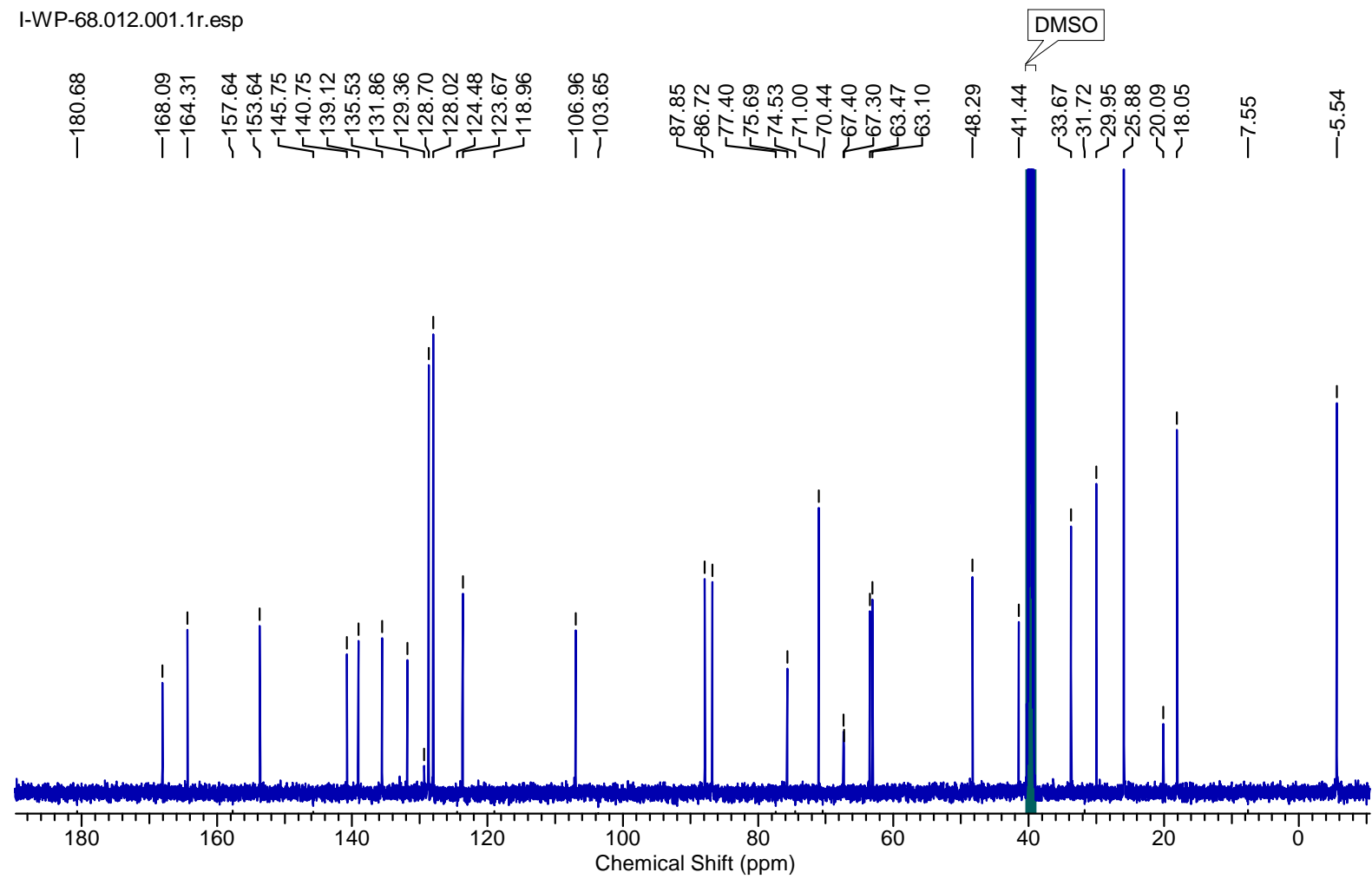


Figure S31. ^{13}C NMR spectrum of compound **23**.

I-WP-68.001.001.1r.esp

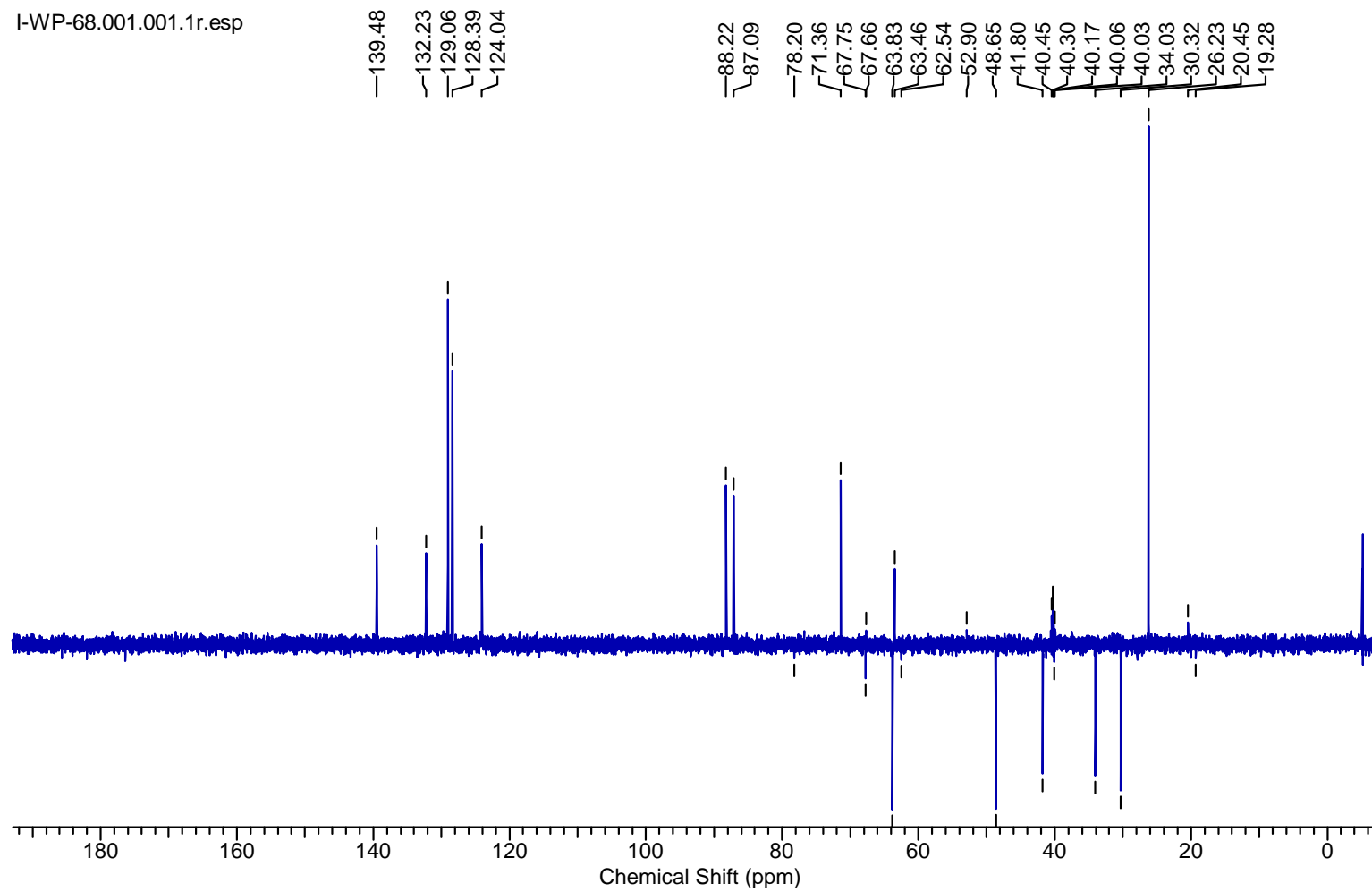


Figure S32. DEPT-135 spectrum of compound **23**.

I-WP-68.004.001.1r.esp

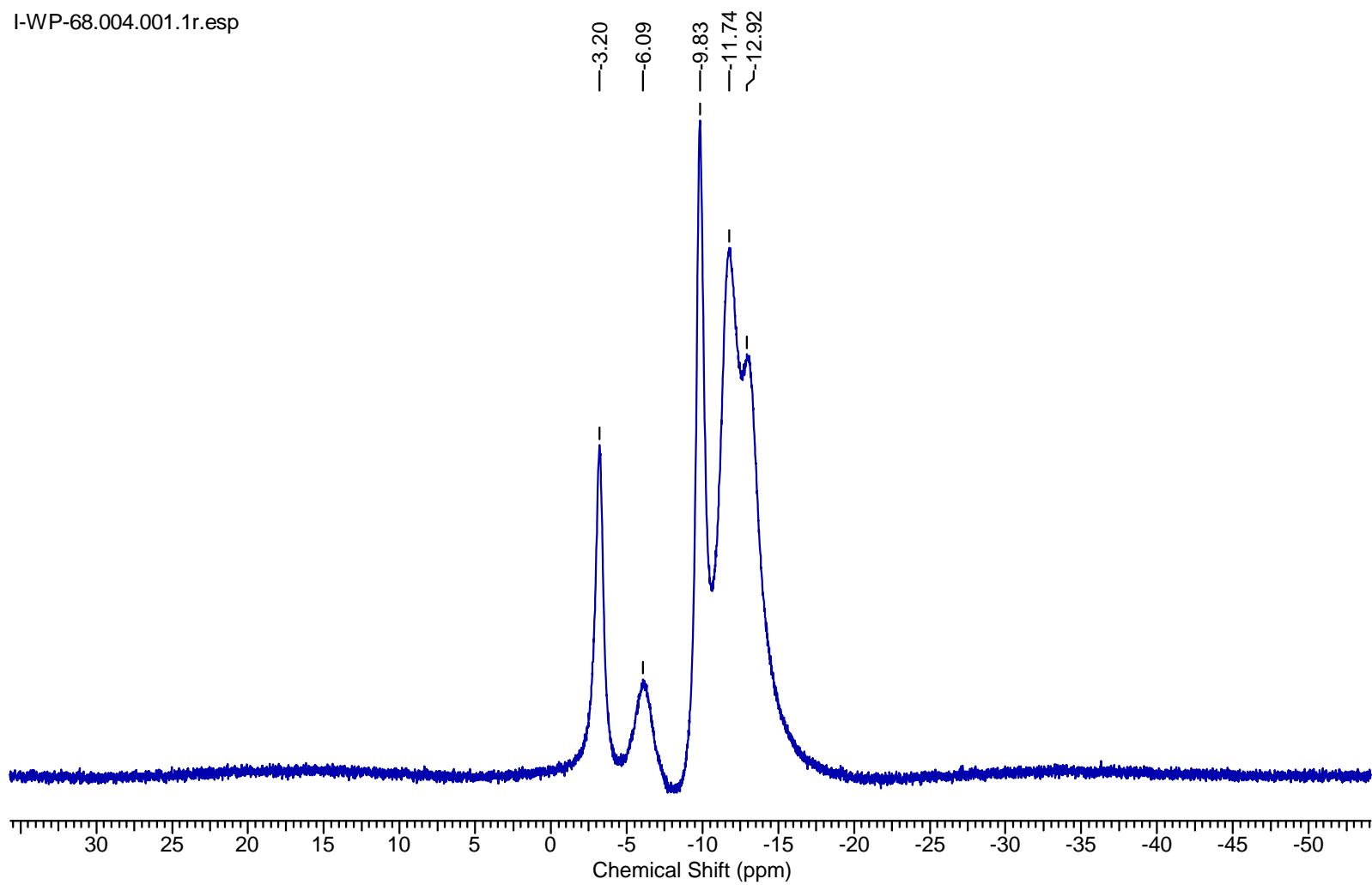


Figure S33. ^{11}B {H BB} NMR spectrum of compound **23**.

I-WP-68.005.001.1r.esp

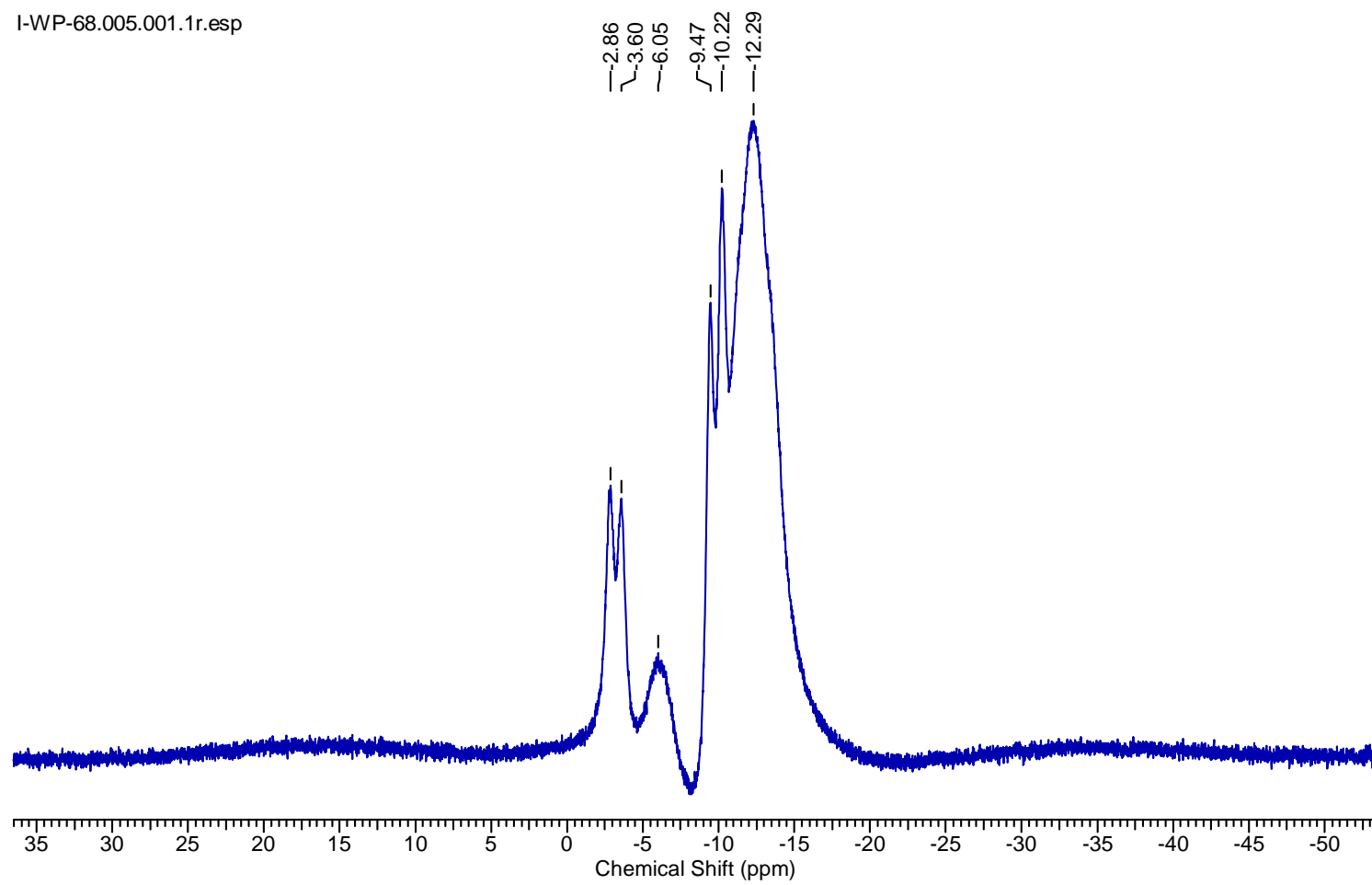


Figure S34. ^{11}B NMR spectrum of compound **23**.

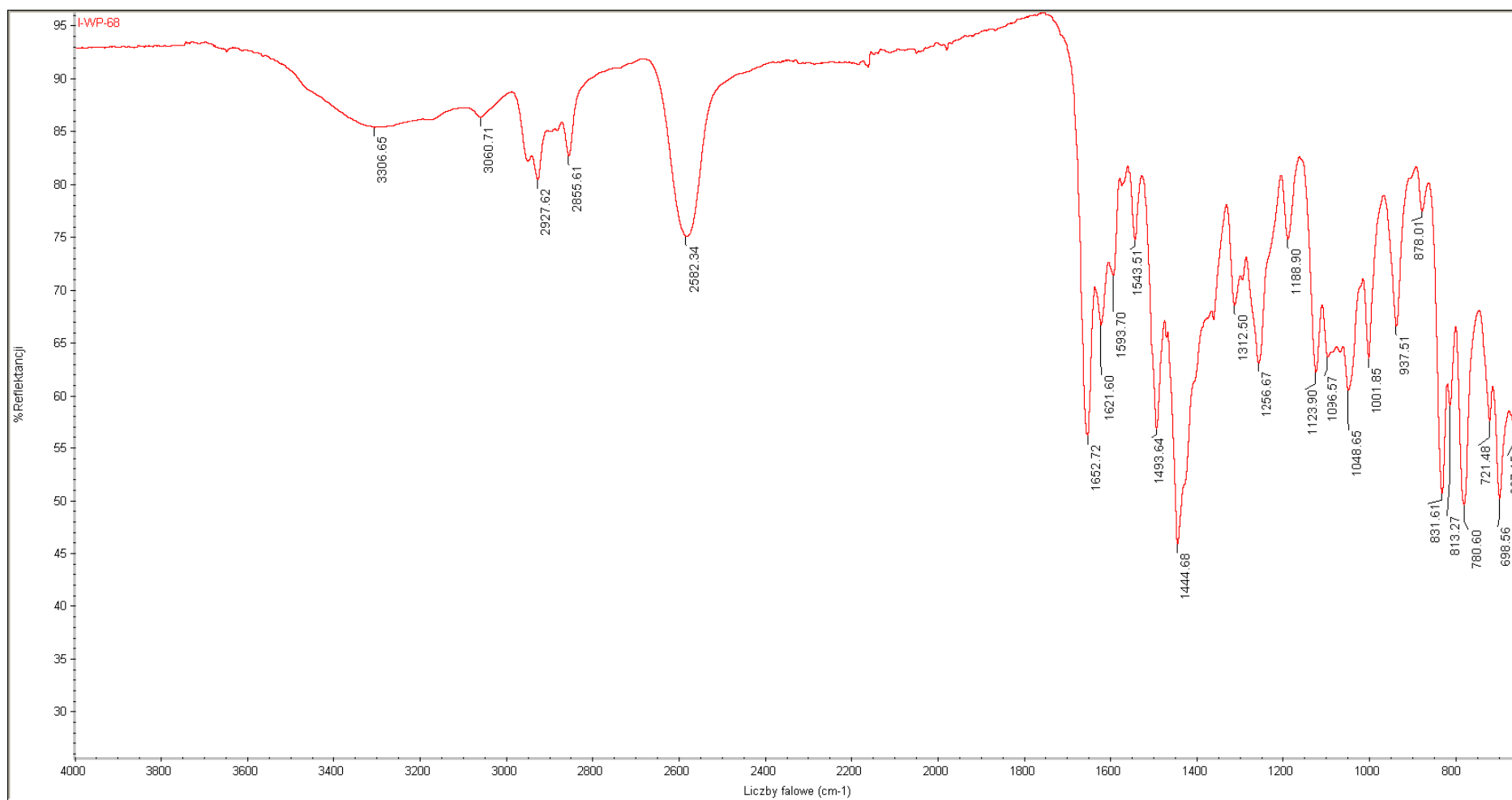
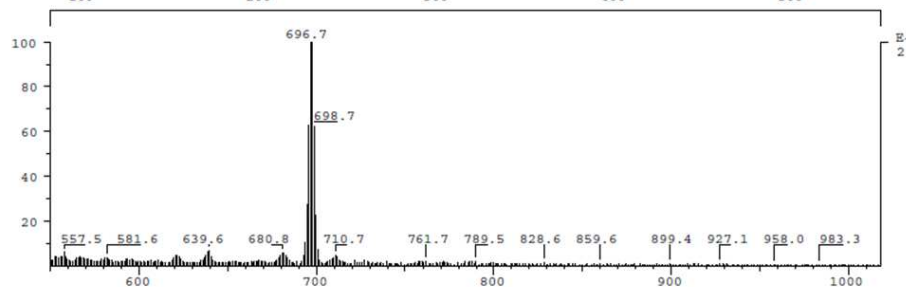
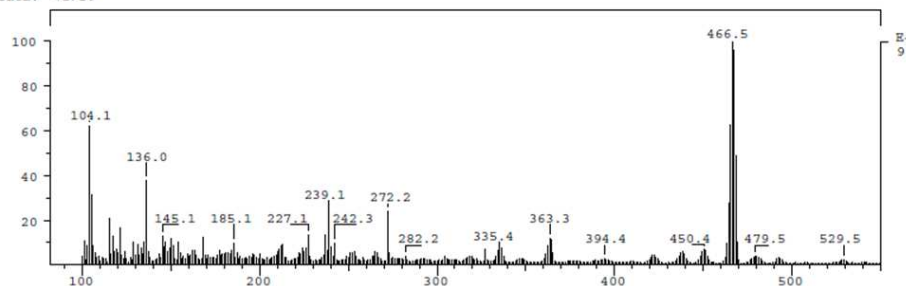


Figure S35. IR spectrum of compound **23**.

SPEC: az087ibm 26-Sep-13 REG : 00:16.9 #9
 Samp: I-WP-68 Start : 10:09:54 10
 Comm: LSI, Cs+ 13 keV, gly
 Mode: FAB +VE +LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ub Client: IBM A.Olejniczak Inlet :
 Base: 466.5 Inten : 925778 Masses: 100 > 1126
 Norm: 466.5 RIC : 19781705 #peaks: 921
 Peak: 1000.00 mmu
 Data: +1>10



SPEC: az087ibm_a 26-Sep-13 REG : 00:16.9 #9
 Samp: I-WP-68 Start : 12:19:07 10
 Comm: LSI, Cs+ 13 keV, gly
 Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ub Client: IBM A.Olejniczak Inlet :
 Base: 695.4 Inten : 300395 Masses: 100 > 1131
 Norm: 695.4 RIC : 10075266 #peaks: 946
 Peak: 1000.00 mmu
 Data: +1>10

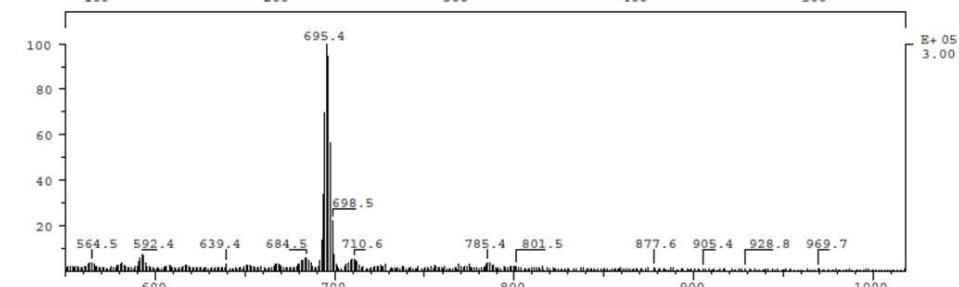
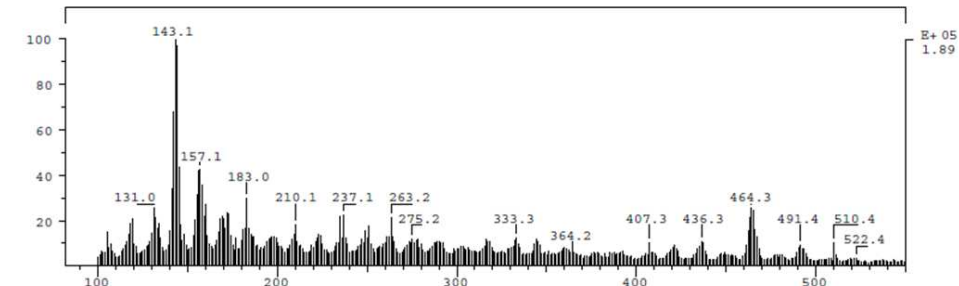


Figure S36. MS-FAB spectra of compound 23.

II-MM-amido-dc-aceton.010.001.1r.esp

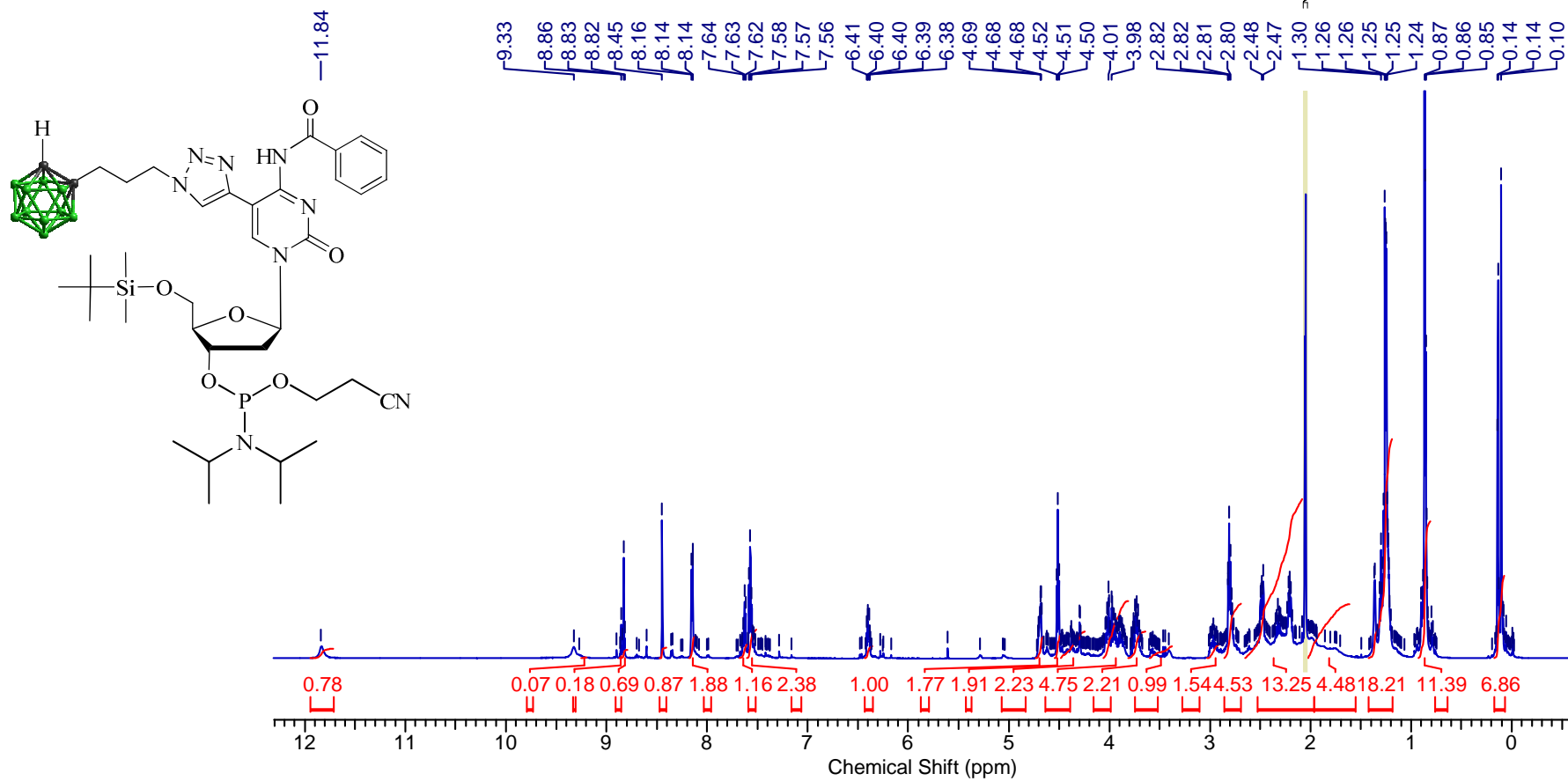


Figure S37. ¹H NMR spectrum of compound 30.

II-MM-amido-dc-aceton.012.001.1r.esp

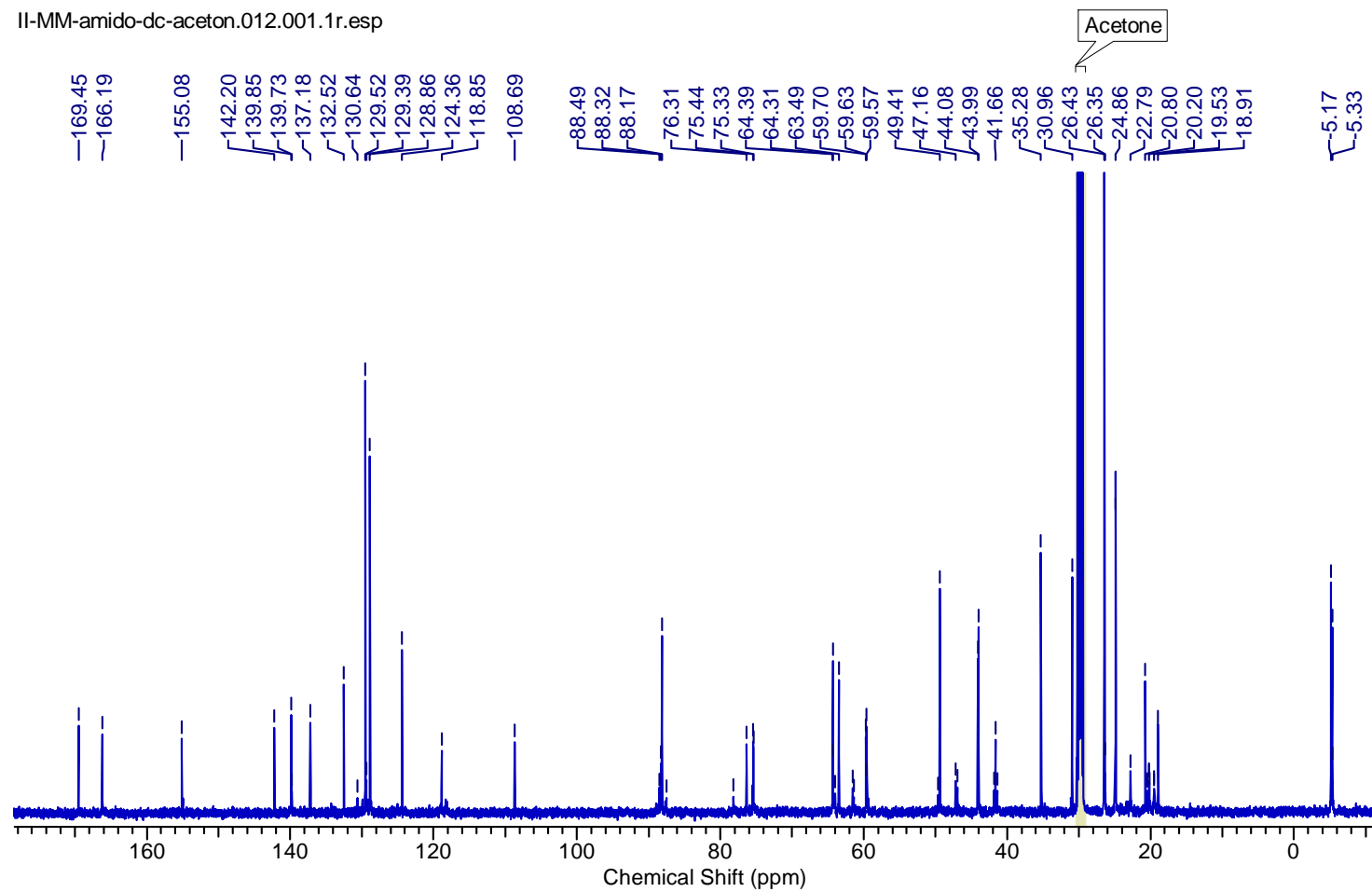


Figure S38. ^{13}C NMR spectrum of compound 30.

II-MM-amido-dc-aceton.013.001.1r.esp

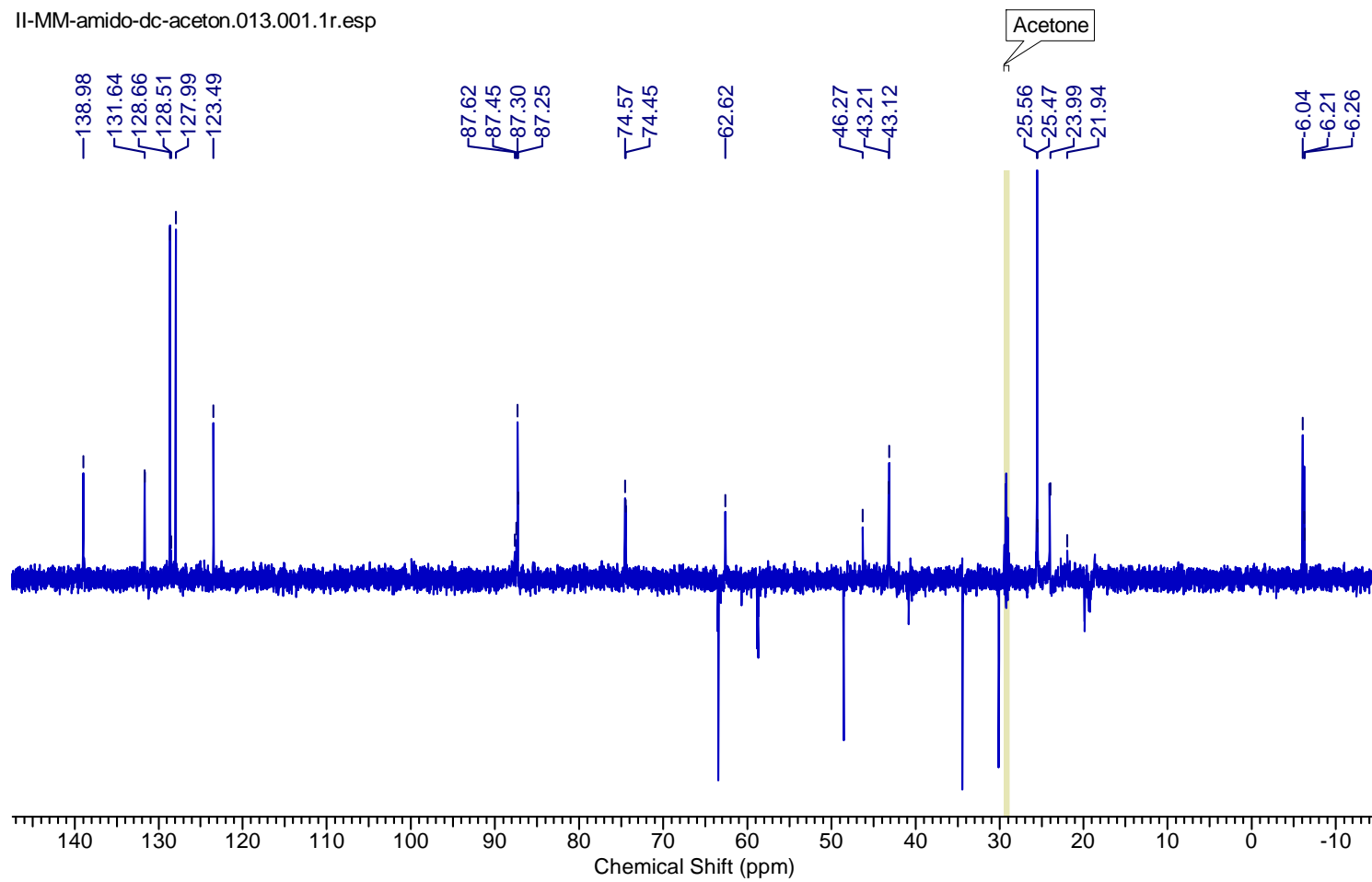


Figure S39. DEPT-135 spectrum of compound **30**.

II-MM-amido-dc-aceton.007.001.1r.esp

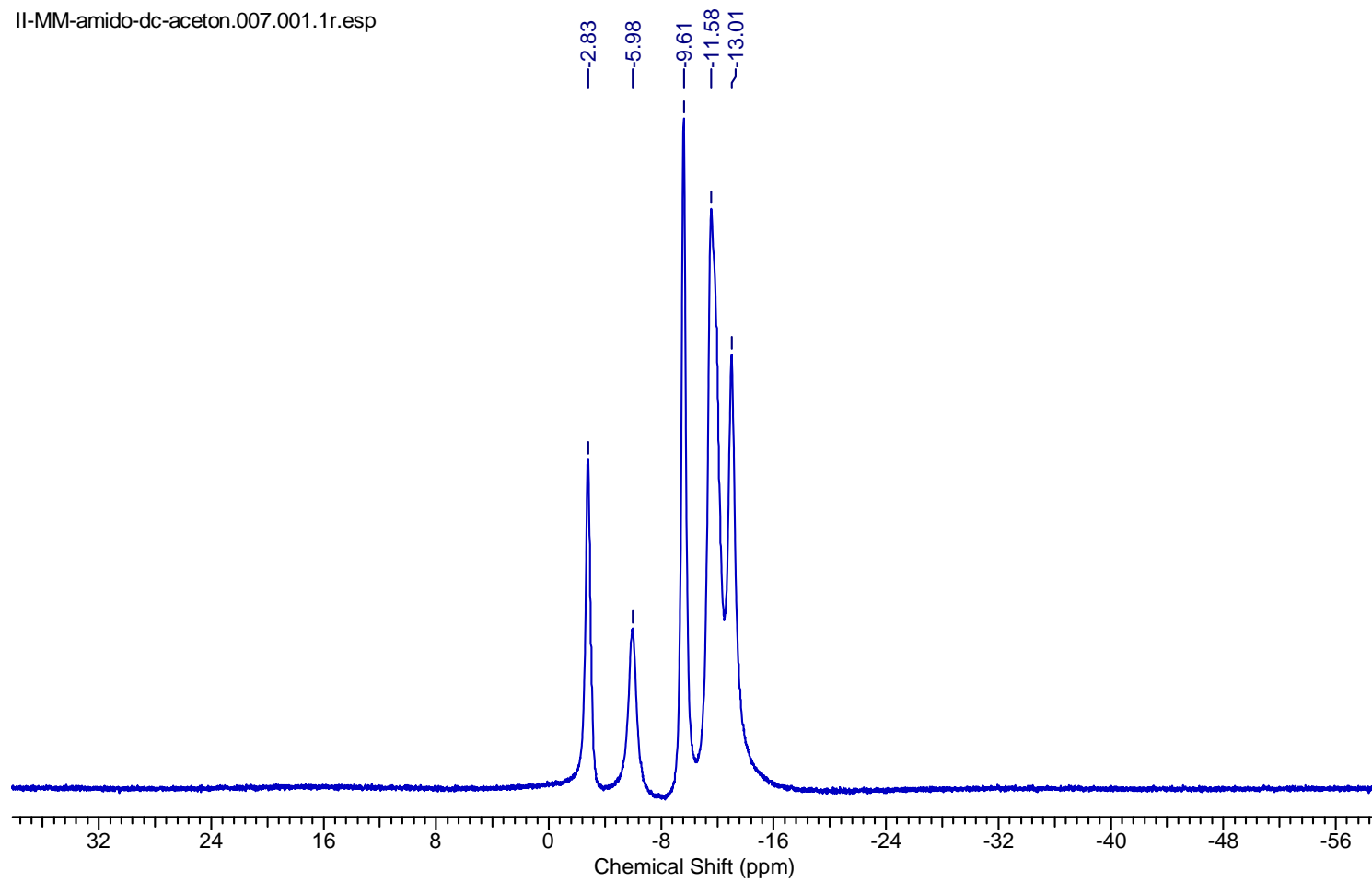


Figure S40. $^{11}\text{B}\{\text{H BB}\}$ NMR spectrum of compound **30**.

II-MM-amido-dc-aceton.008.001.1r.esp

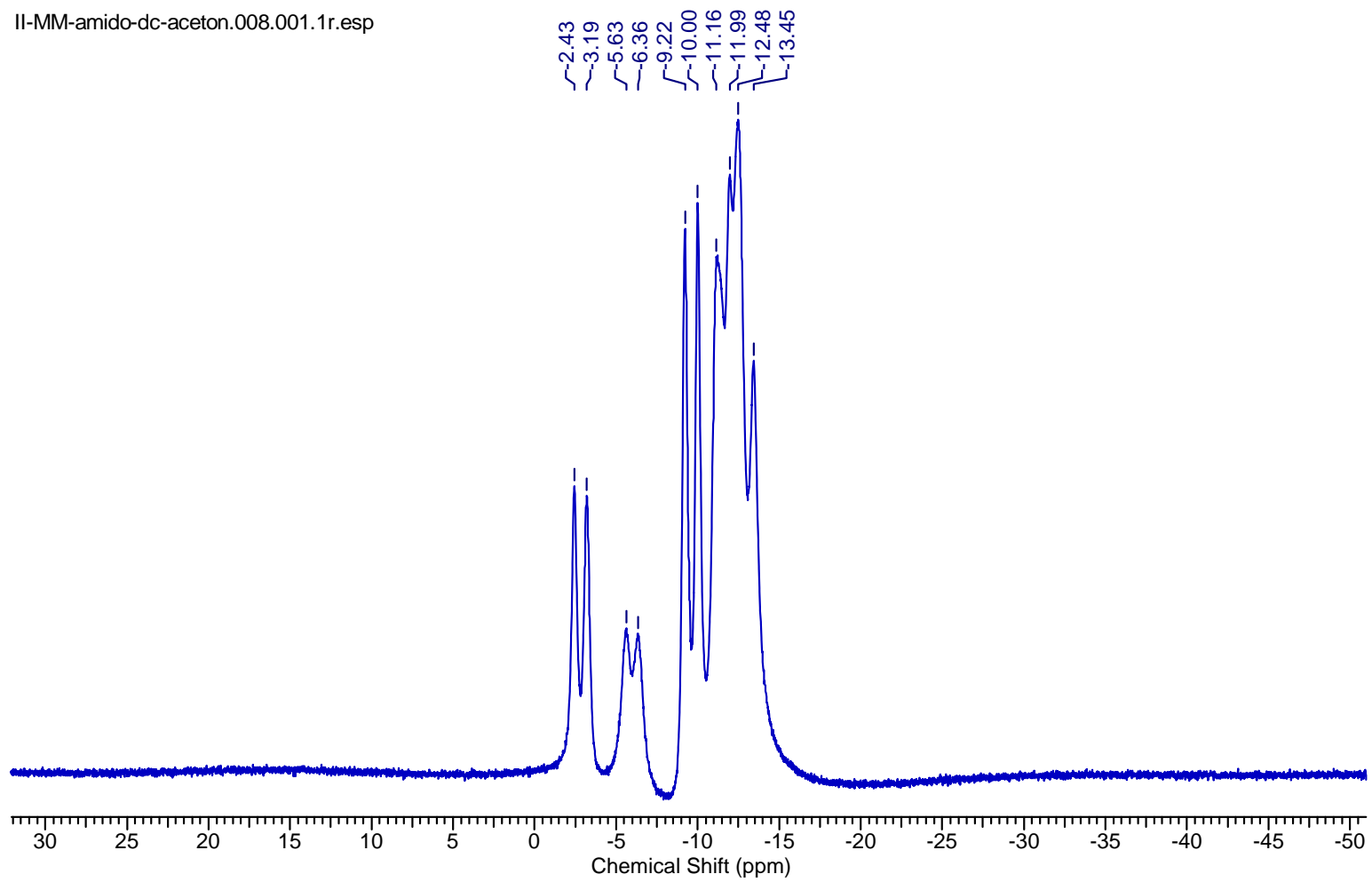


Figure S41. ^{11}B NMR spectrum of compound **30**

II-MM-amido-dc-aceton.001.001.1r.esp

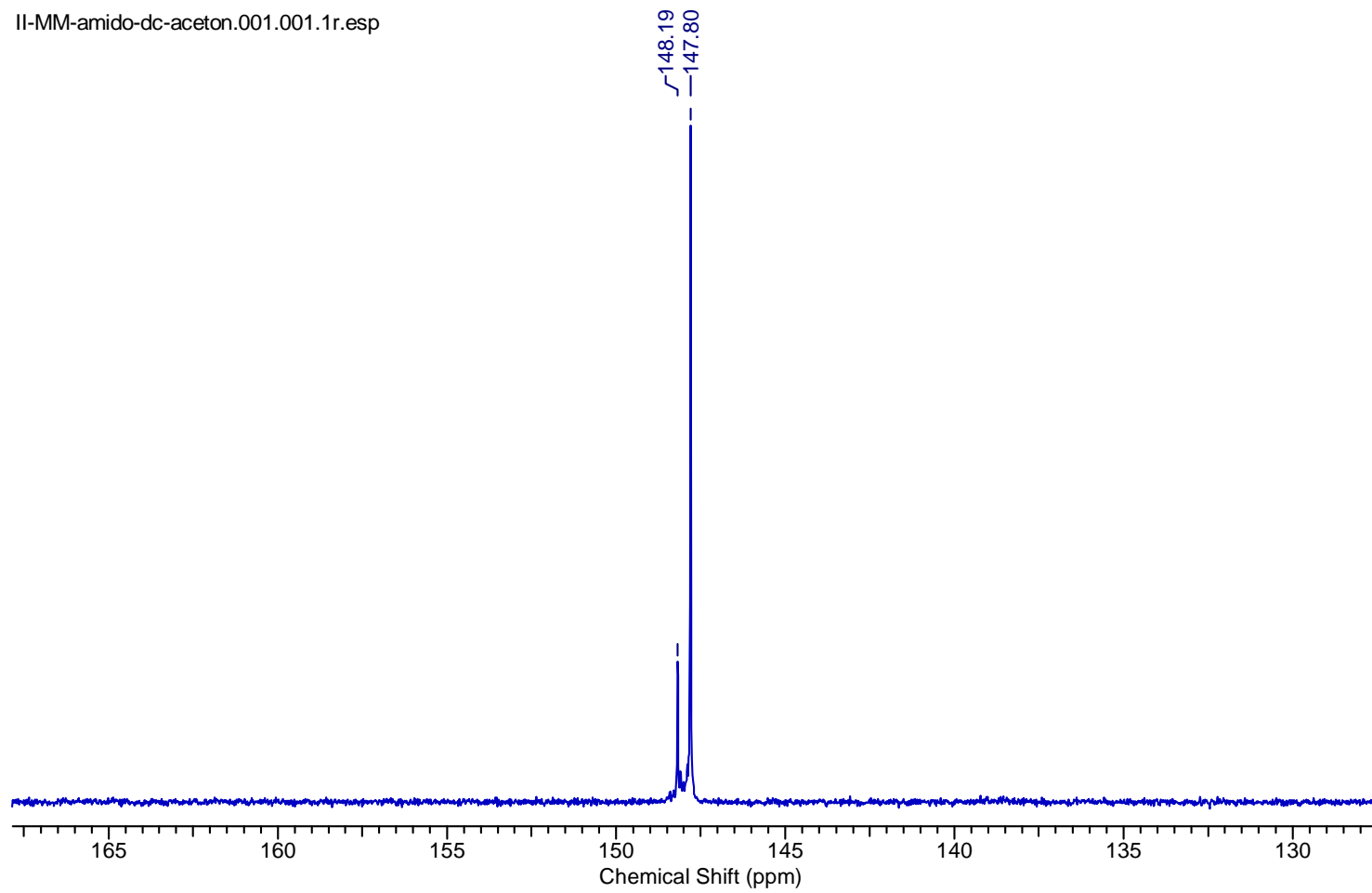


Figure S42. ^{31}P NMR spectrum of compound **30**.

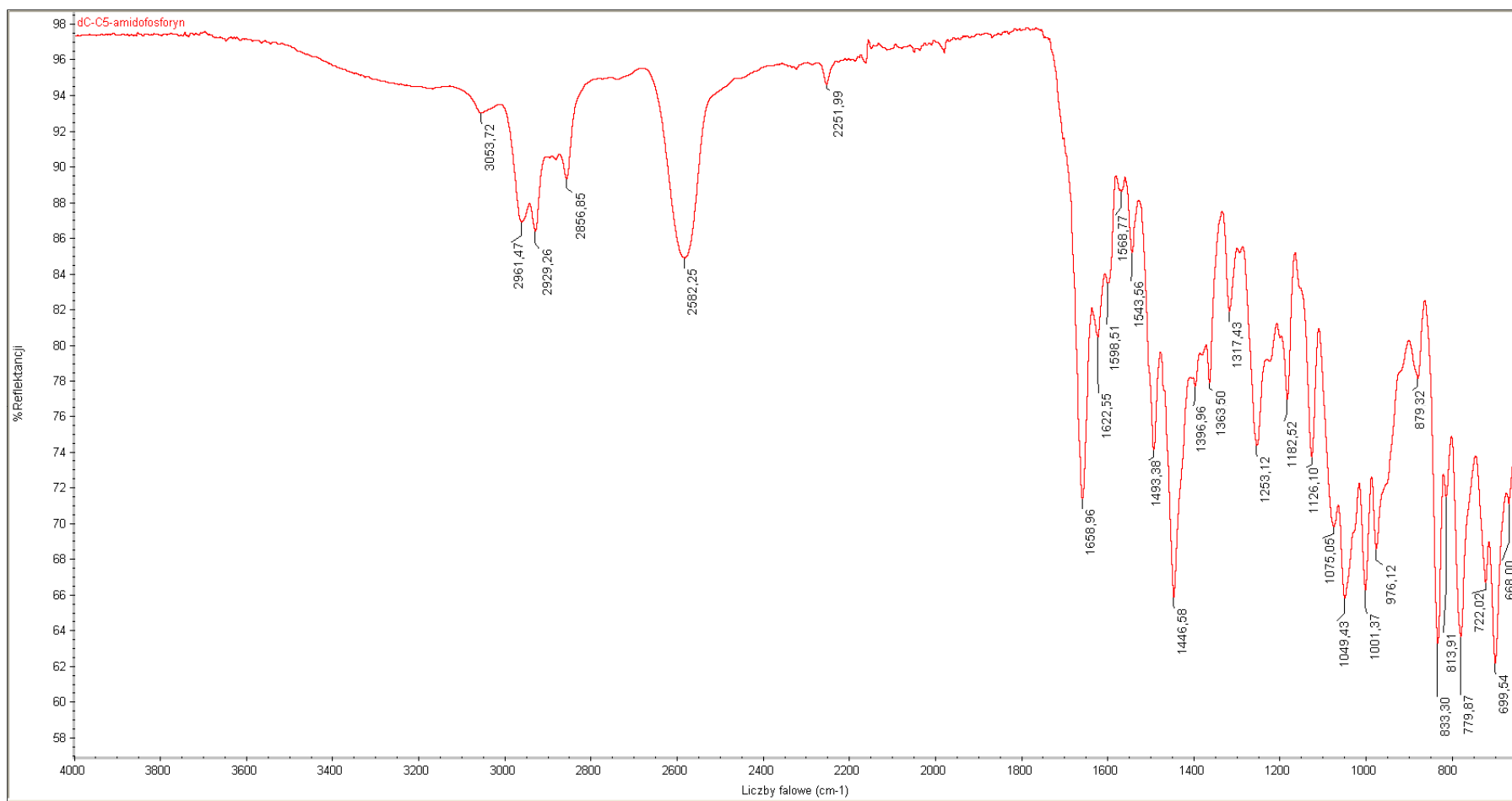


Figure S43. IR spectrum of compound **30**.

SPEC: az468ibm_b 23-Dec-13 REG : 00:16.9 #9
Samp: dC-amido Start : 11:22:01 10
Comm: LSI, Cs+ 13 keV, nba
Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBMiM PAN Lodz
Oper: ew Client: IBM A.Olejniczak Inlet :
Base: 153.0 Inten : 2571237 Masses: 100 > 1117
Norm: 153.0 RIC : 19825290 #peaks: 1008
Peak: 1000.00 mmu
Data: +1>10

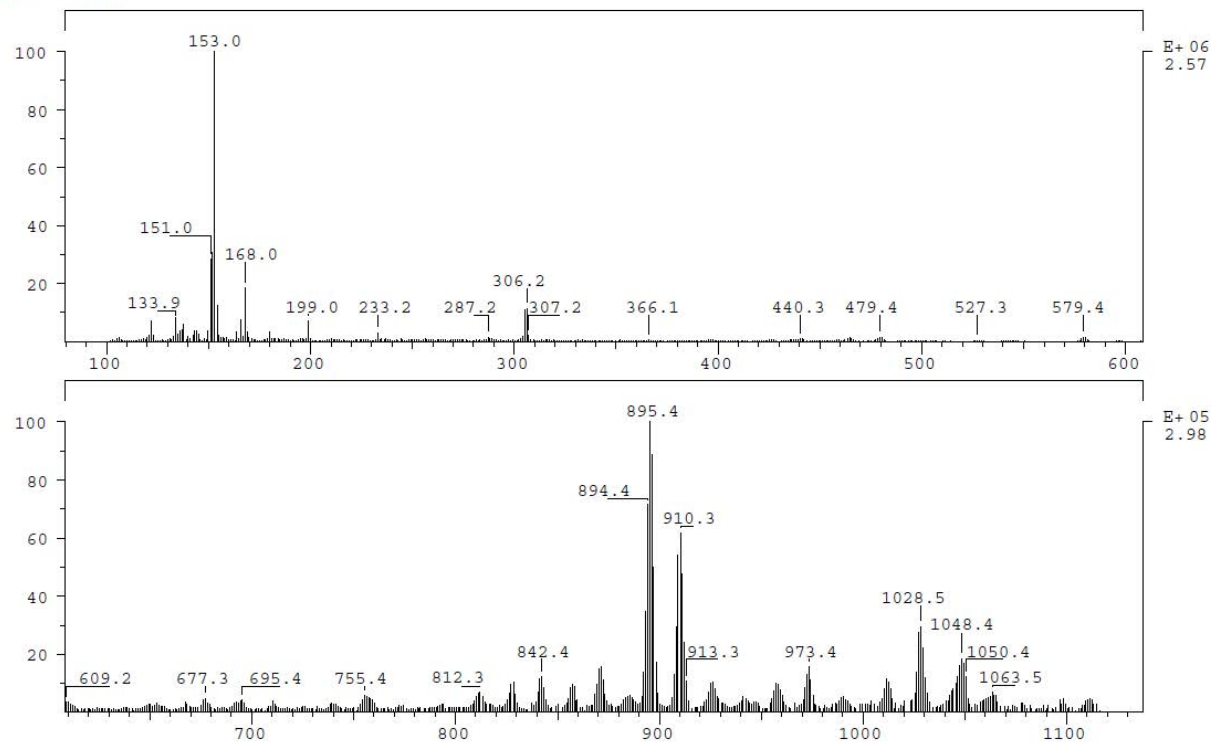


Figure S44. MS-FAB spectrum of compound 30.

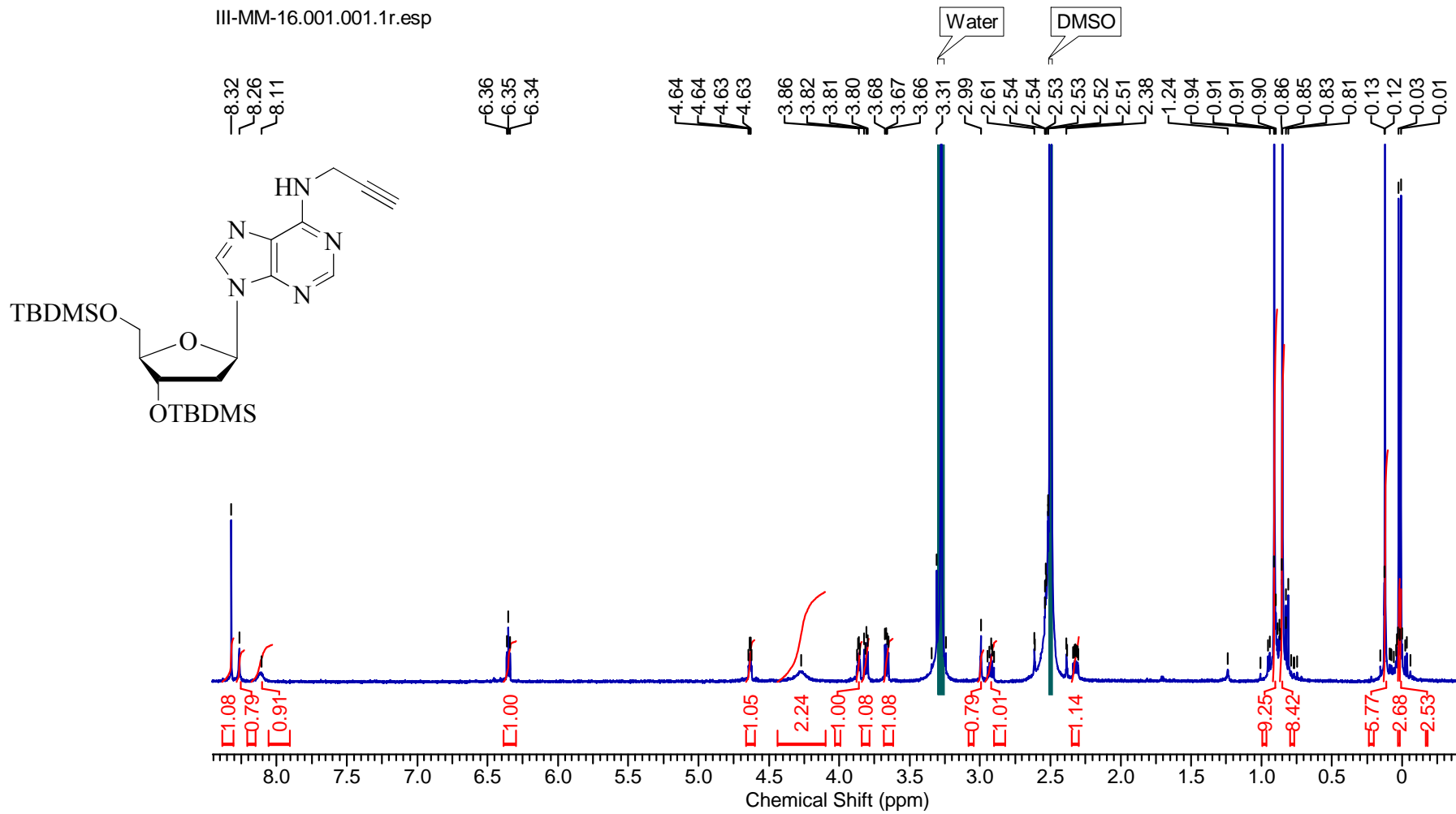


Figure S45. ^1H NMR spectrum of compound 12.

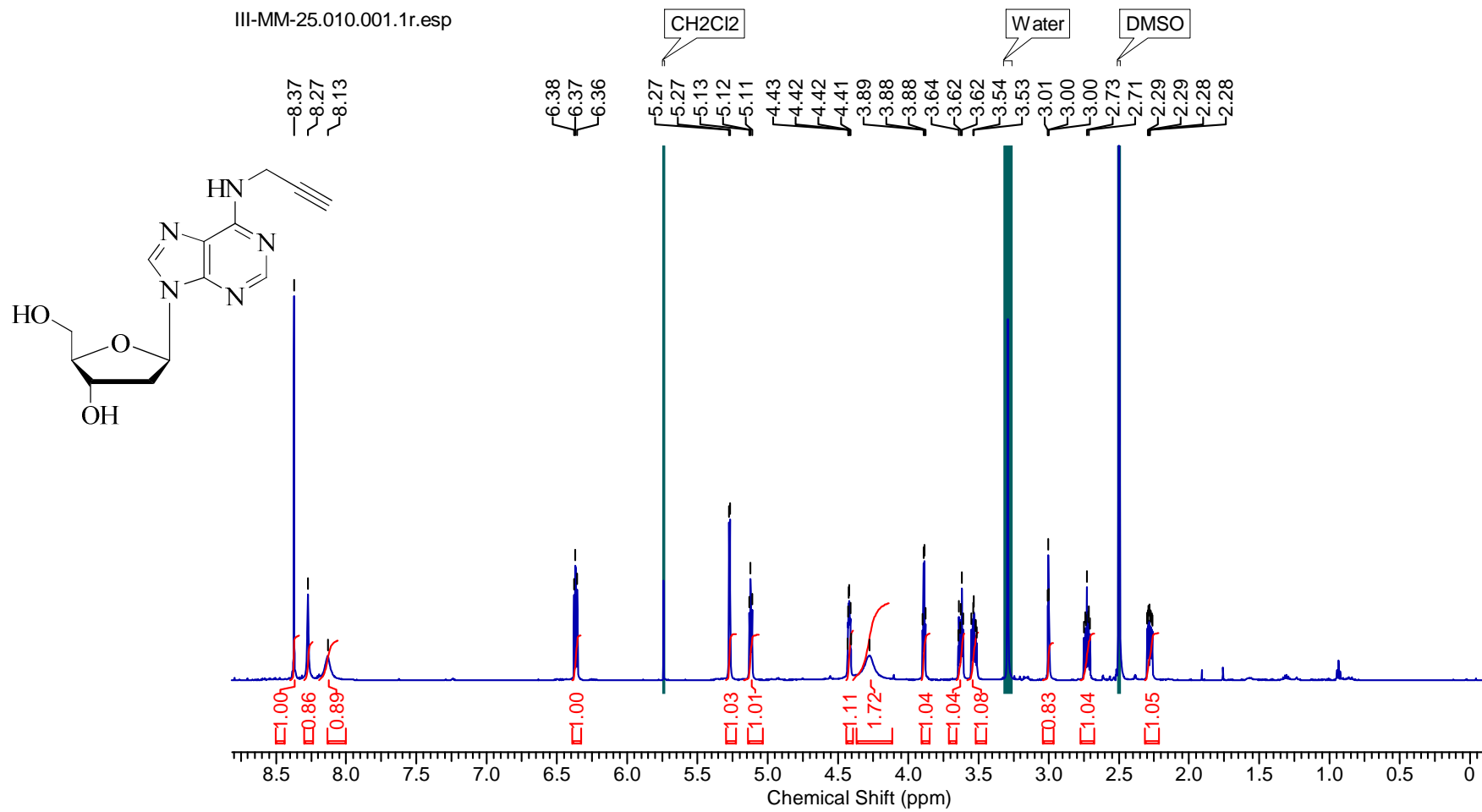


Figure S46. ^1H NMR spectrum of compound 13.

III-MM-40.011.001.1r.esp

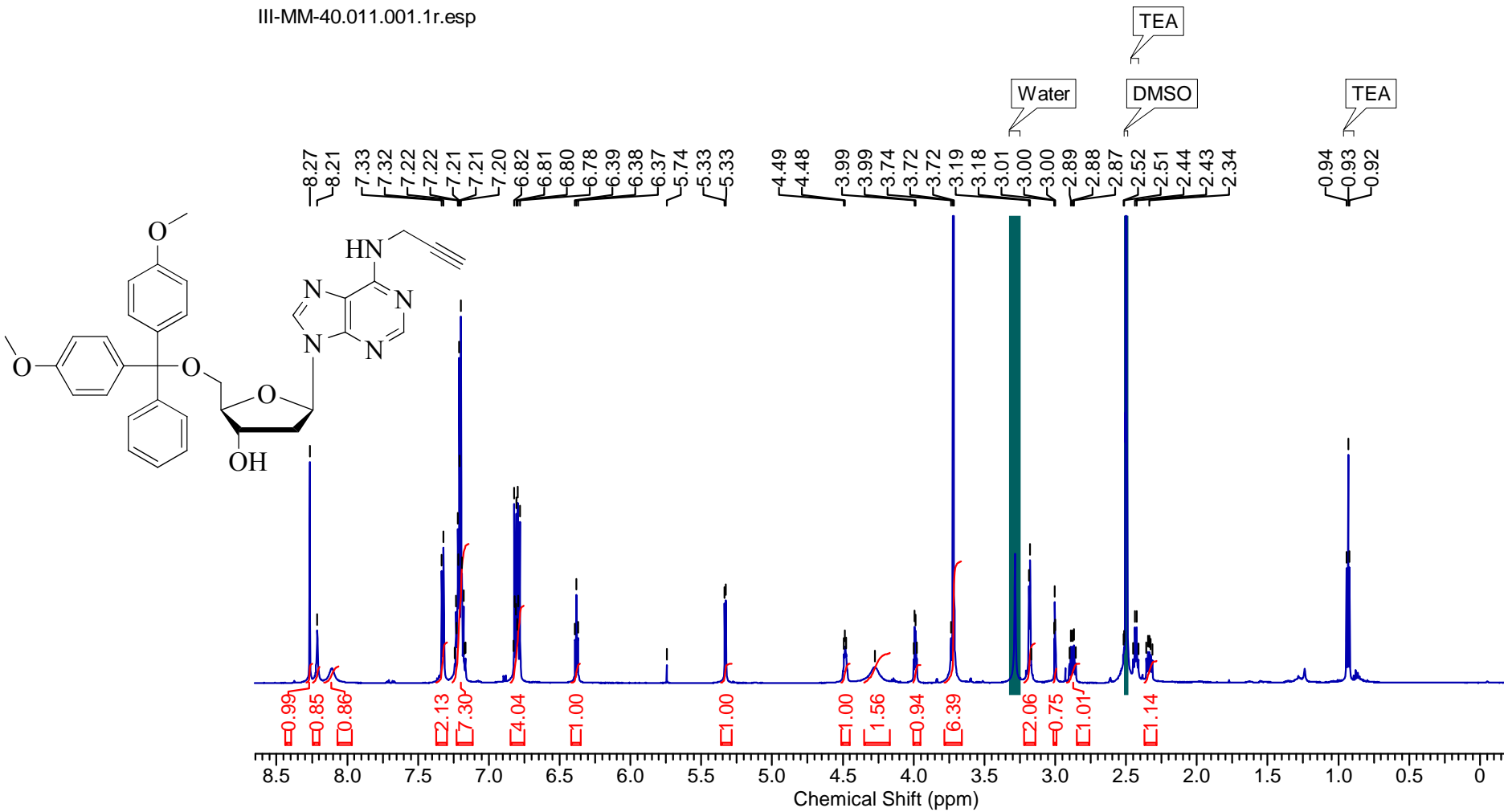


Figure S47. ^1H NMR spectrum of compound 14.

III-MM-40.020.001.1r.esp

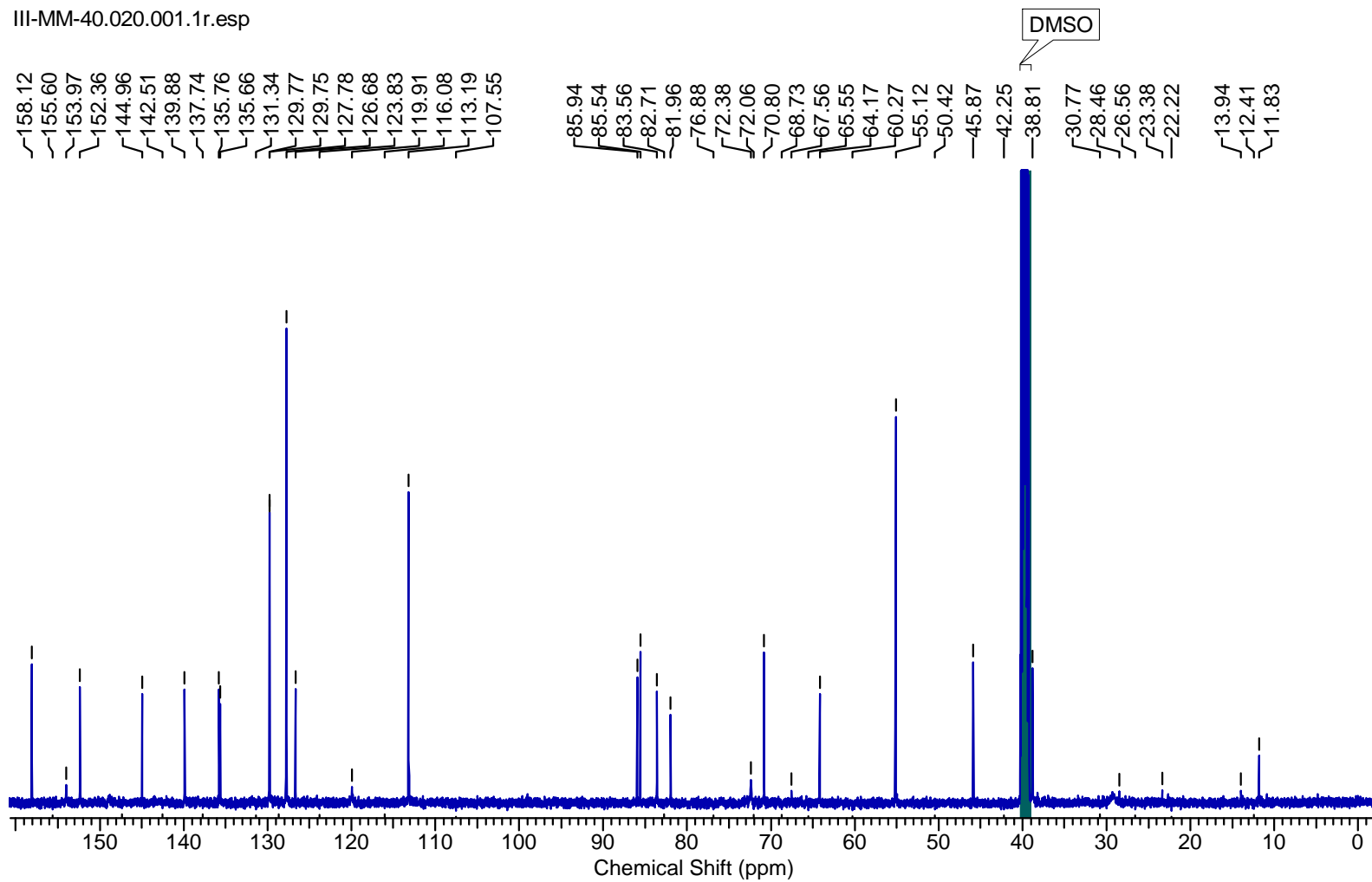


Figure S48. ^{13}C NMR spectrum of compound 14.

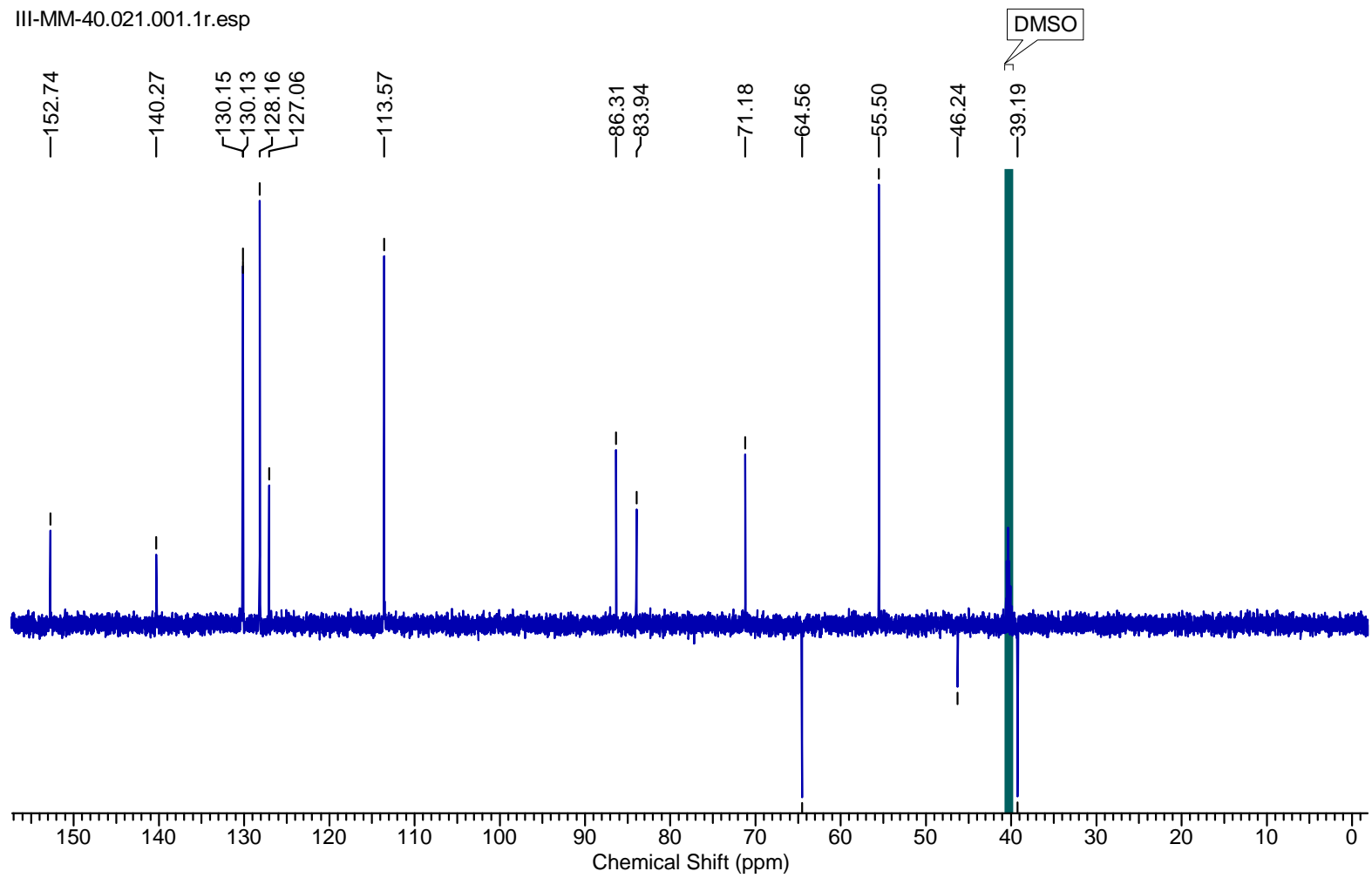


Figure S49. DEPT-135 spectrum of compound **14**.

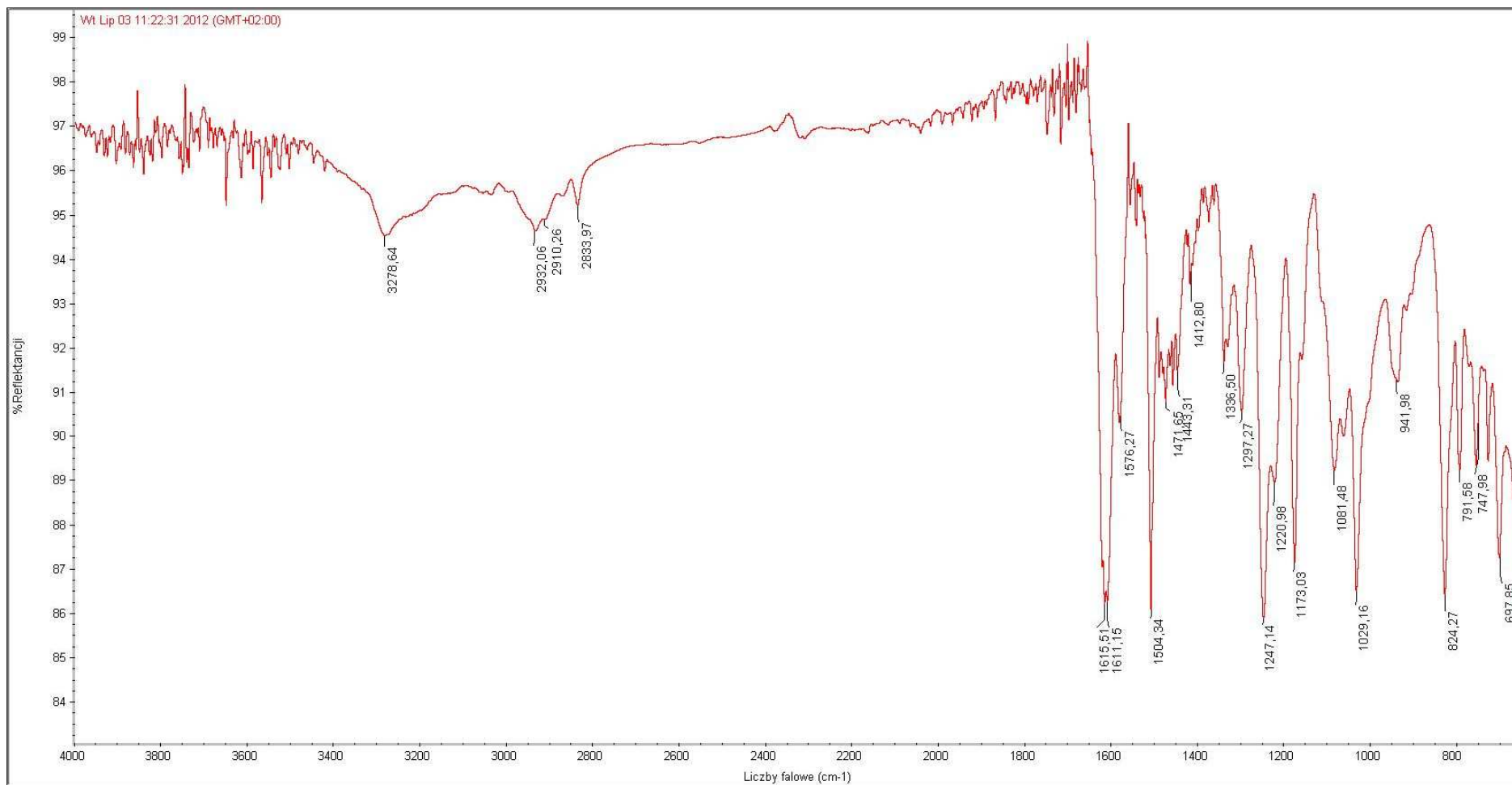
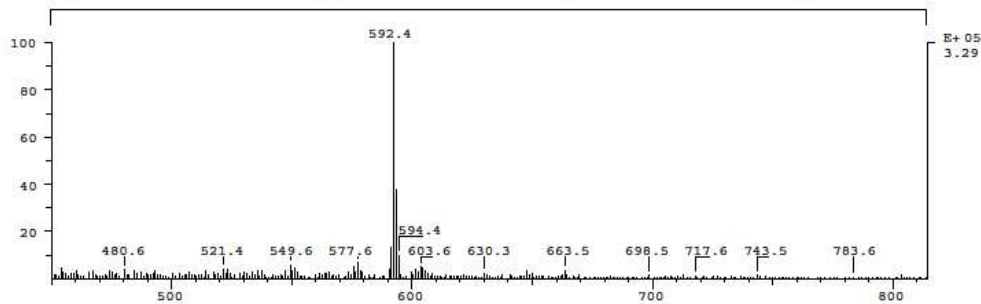
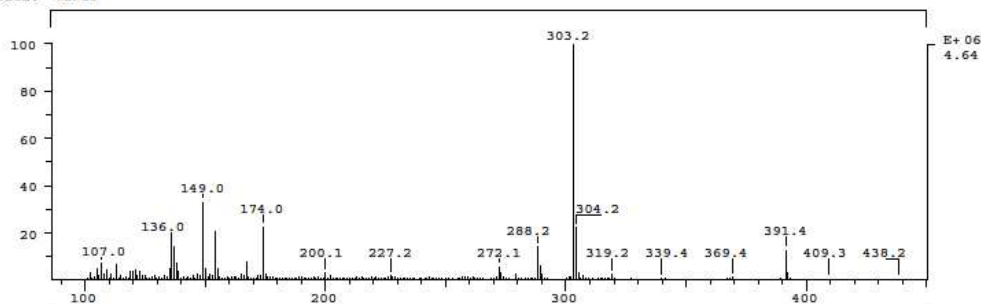


Figure S50. IR spectrum of compound **14**.

SPEC: ax6611bm_a 27-Jun-12 REG : 00:16.4 #9
 Samp: III-MM-40 Start : 13:46:07 10
 Comm: LSI, Cs+ 13 keV, nba
 Mode: FAB +VE +LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ed Client: IBM A.Olejniczak Inlet :
 Base: 303.2 Inten : 4635556 Masses: 100 > 1000
 Norm: 303.2 RIC : 28939076 #peaks: 819
 Peak: 1000.00 mmu
 Data: +1>10



SPEC: ax6611bm 27-Jun-12 REG : 00:16.4 #9
 Samp: III-MM-40 Start : 13:42:19 10
 Comm: LSI, Cs+ 13 keV, nba
 Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ed Client: IBM A.Olejniczak Inlet :
 Base: 152.9 Inten : 946679 Masses: 100 > 1000
 Norm: 152.9 RIC : 7047203 #peaks: 728
 Peak: 1000.00 mmu
 Data: +1>10

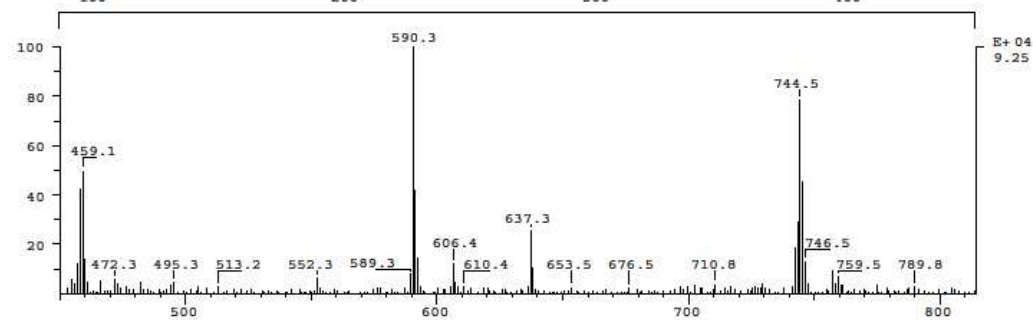
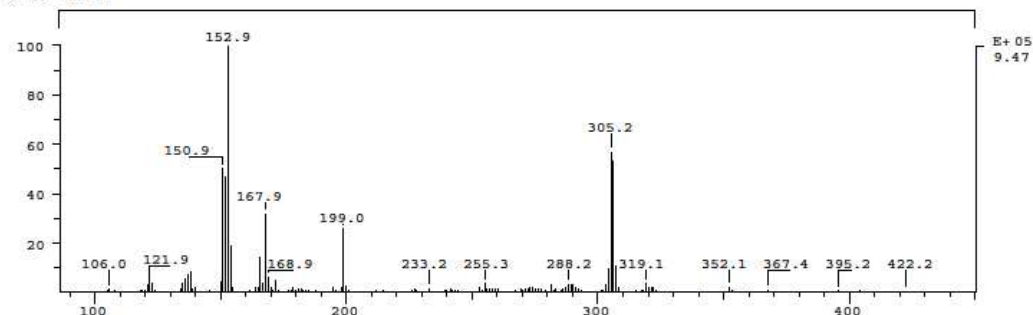


Figure S51. MS-FAB spectra of compound 14.

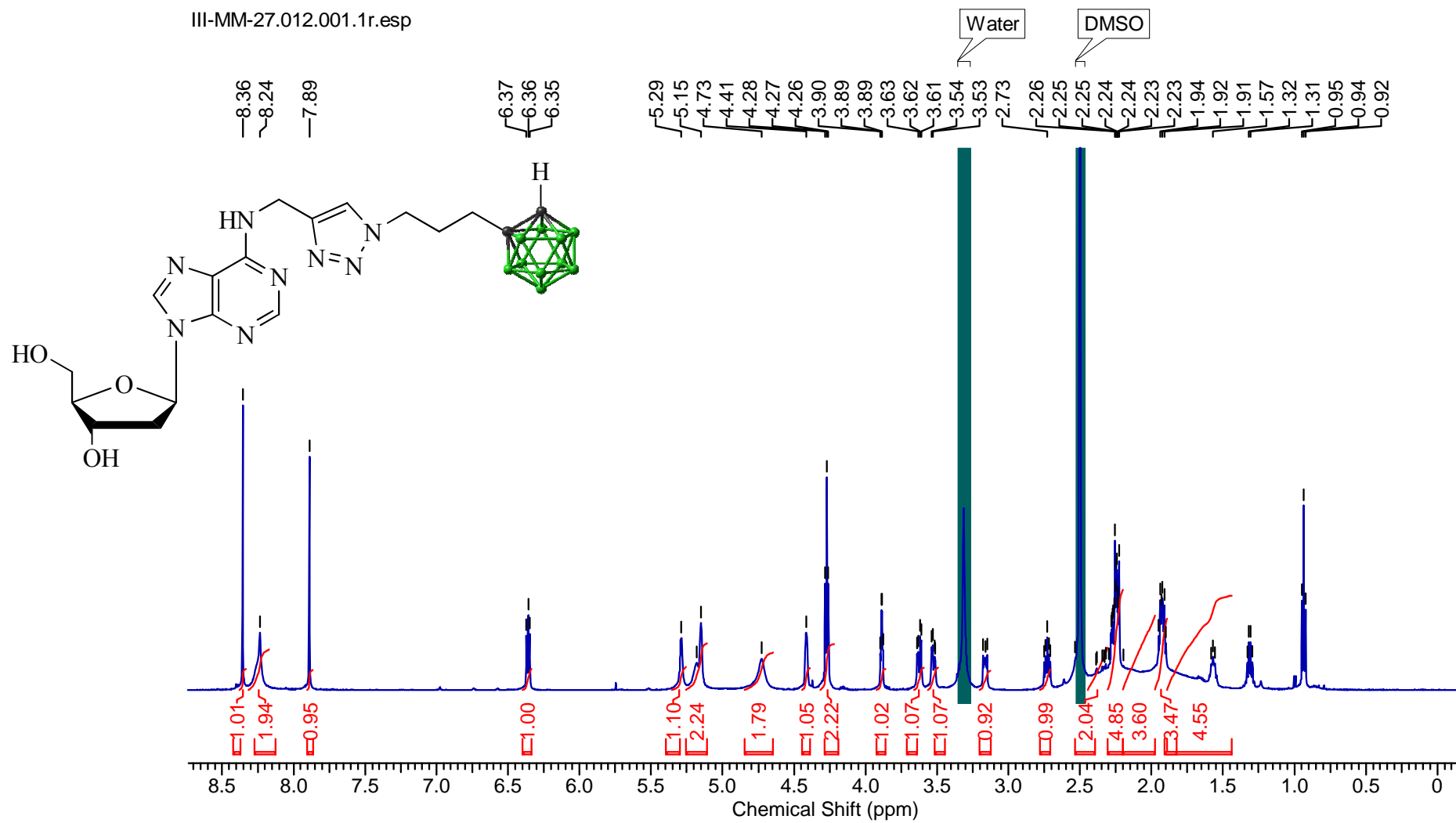


Figure S52. ¹H NMR spectrum of compound 24.

III-MM-27.010.001.1r.esp

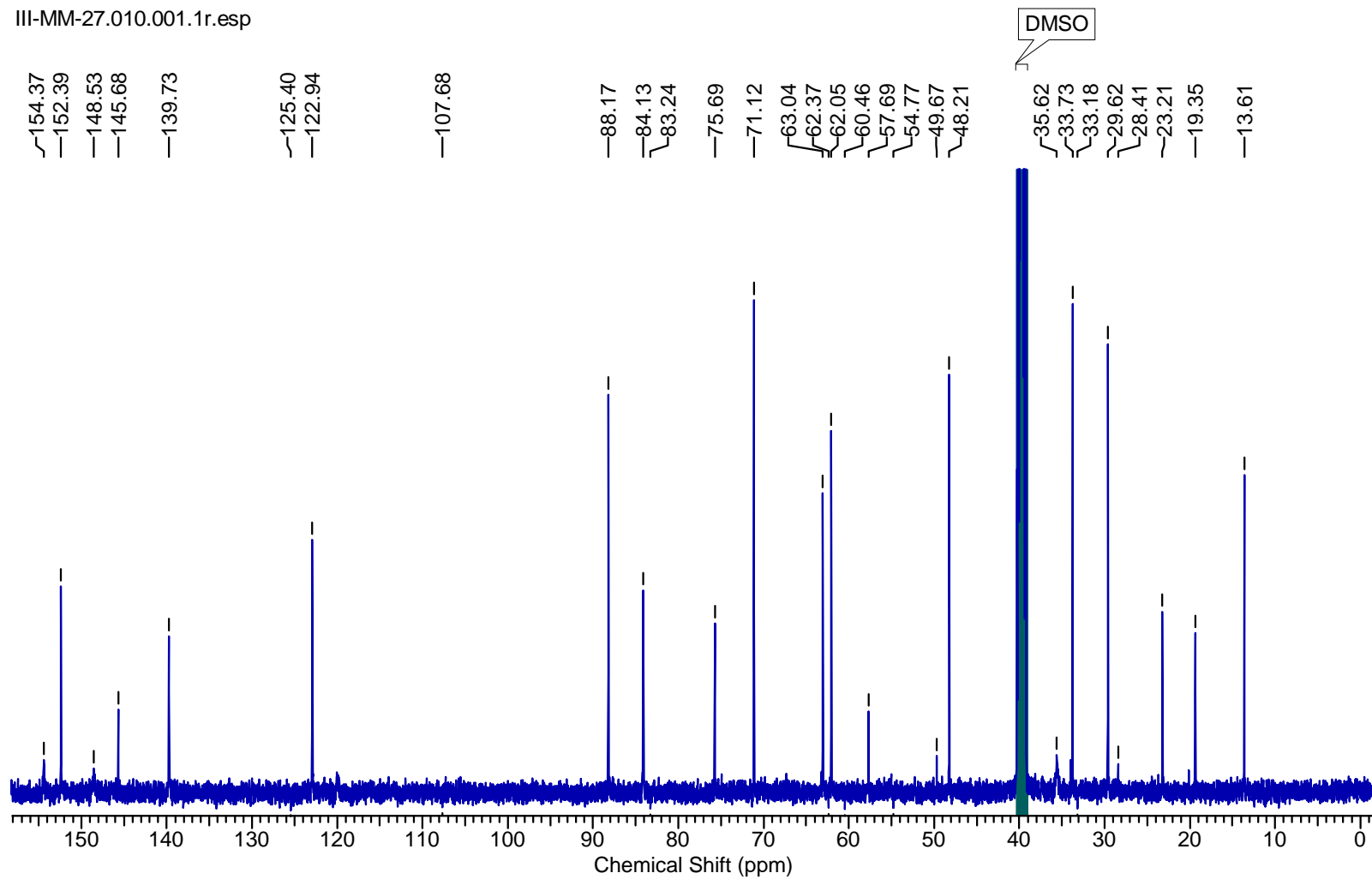


Figure S53. ^{13}C NMR spectrum of compound 24.

III-MM-27.011.001.1r.esp

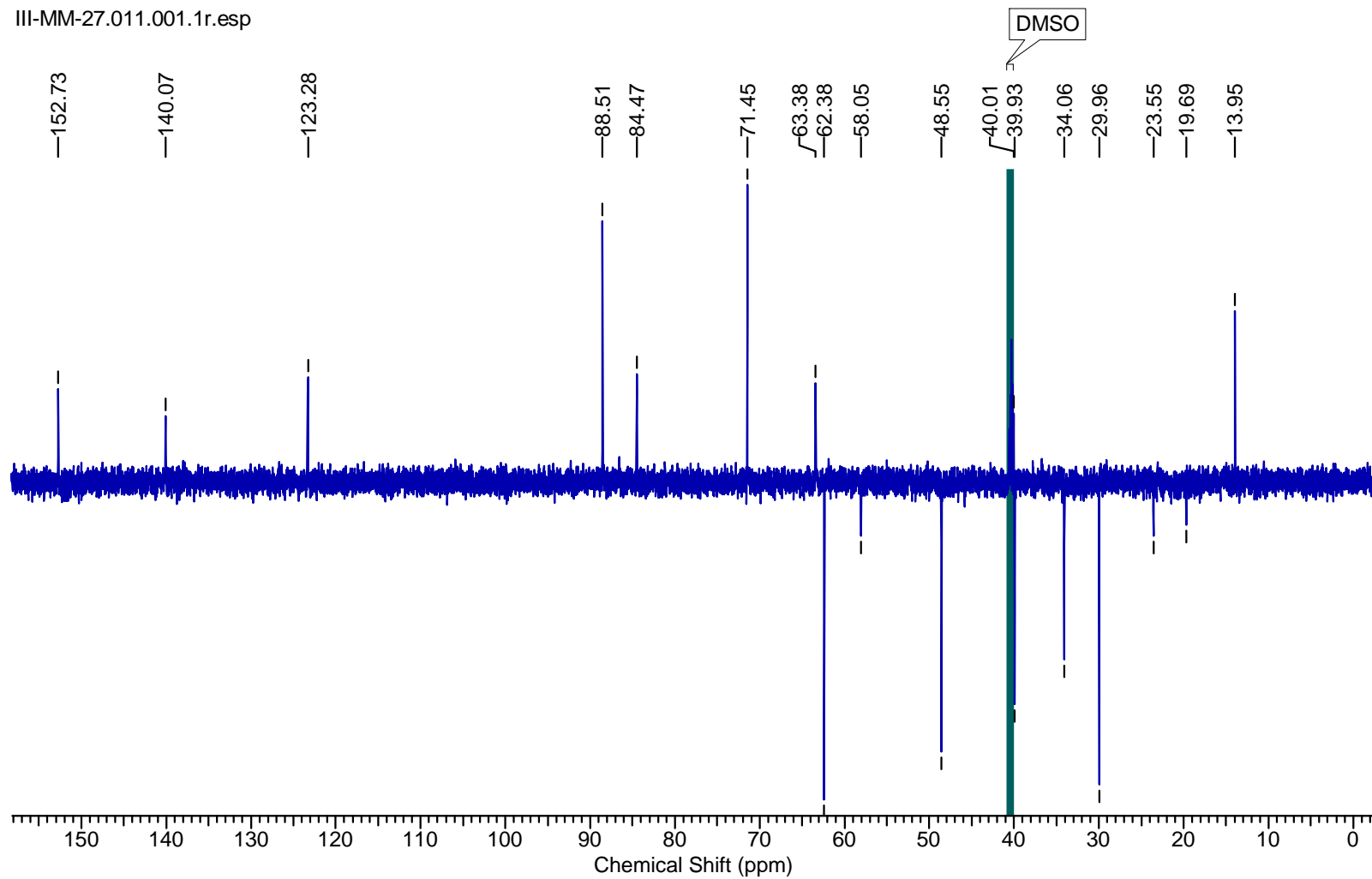


Figure S54. DEPT-135 spectrum of compound **24**.

III-MM-27.003.001.1r.esp

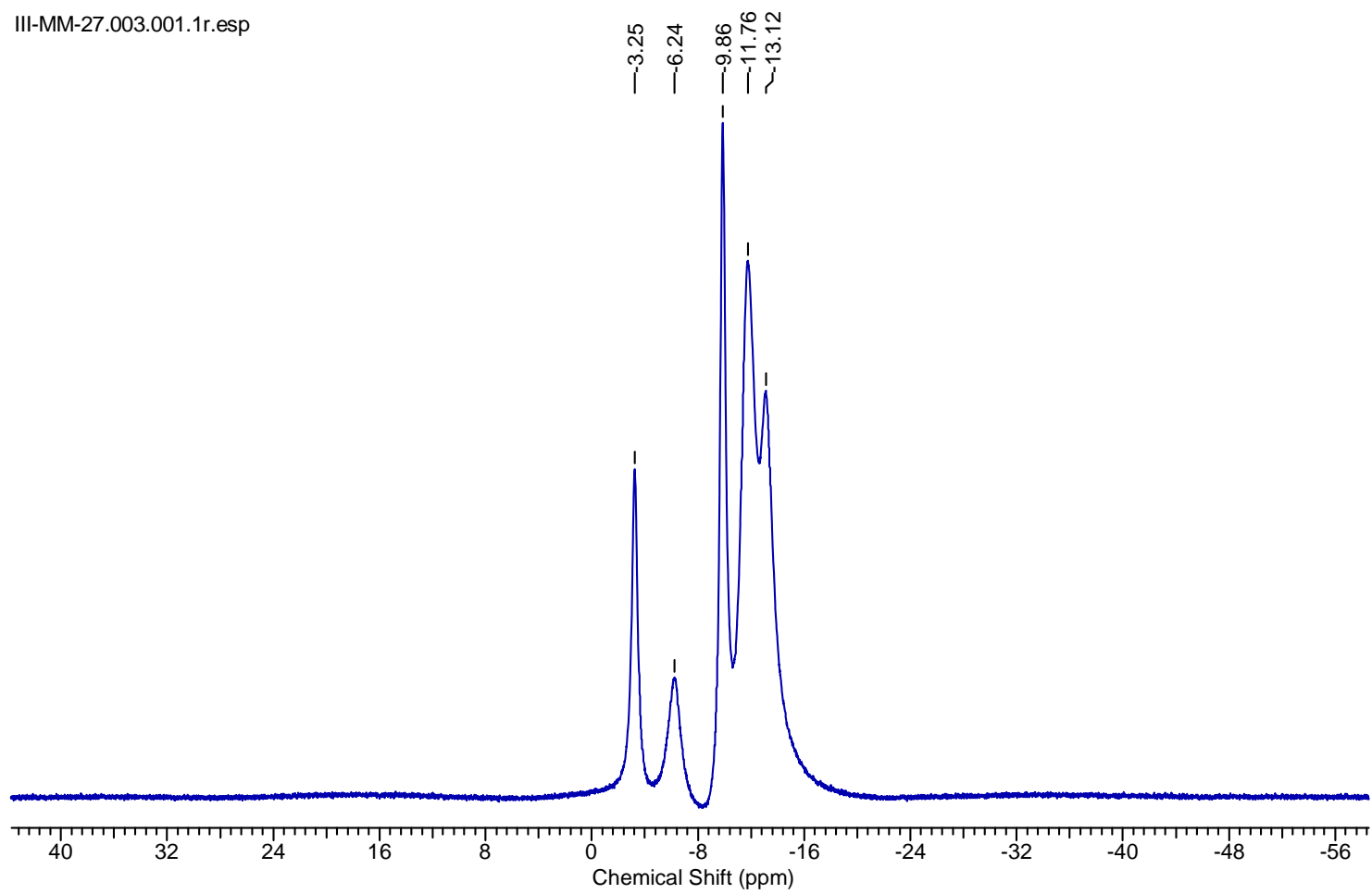


Figure S55. $^{11}\text{B}\{^1\text{H BB}\}$ NMR spectrum of compound **24**.

III-MM-27.004.001.1r.esp

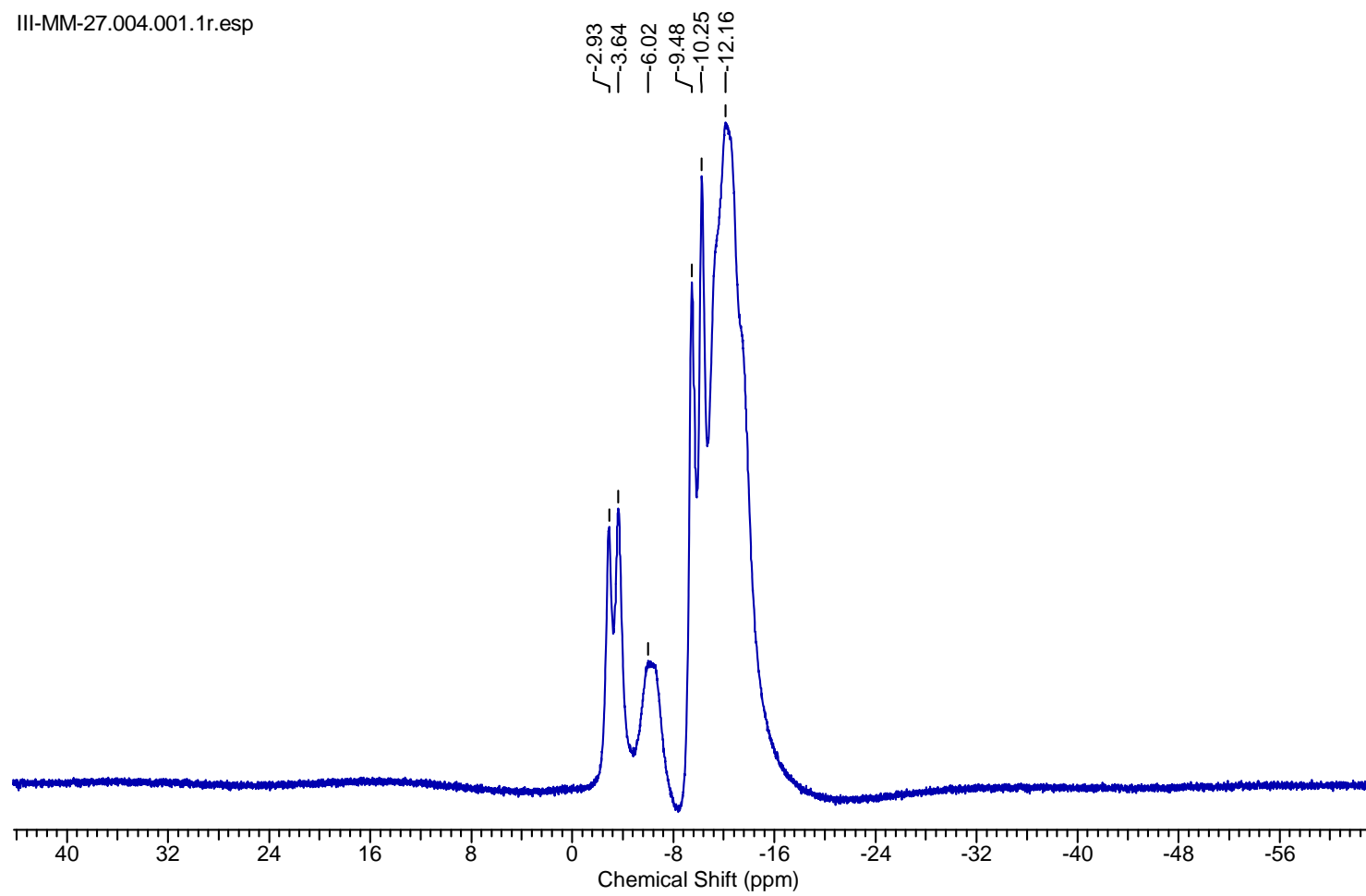


Figure S56. ^{11}B NMR spectrum of compound **24**.

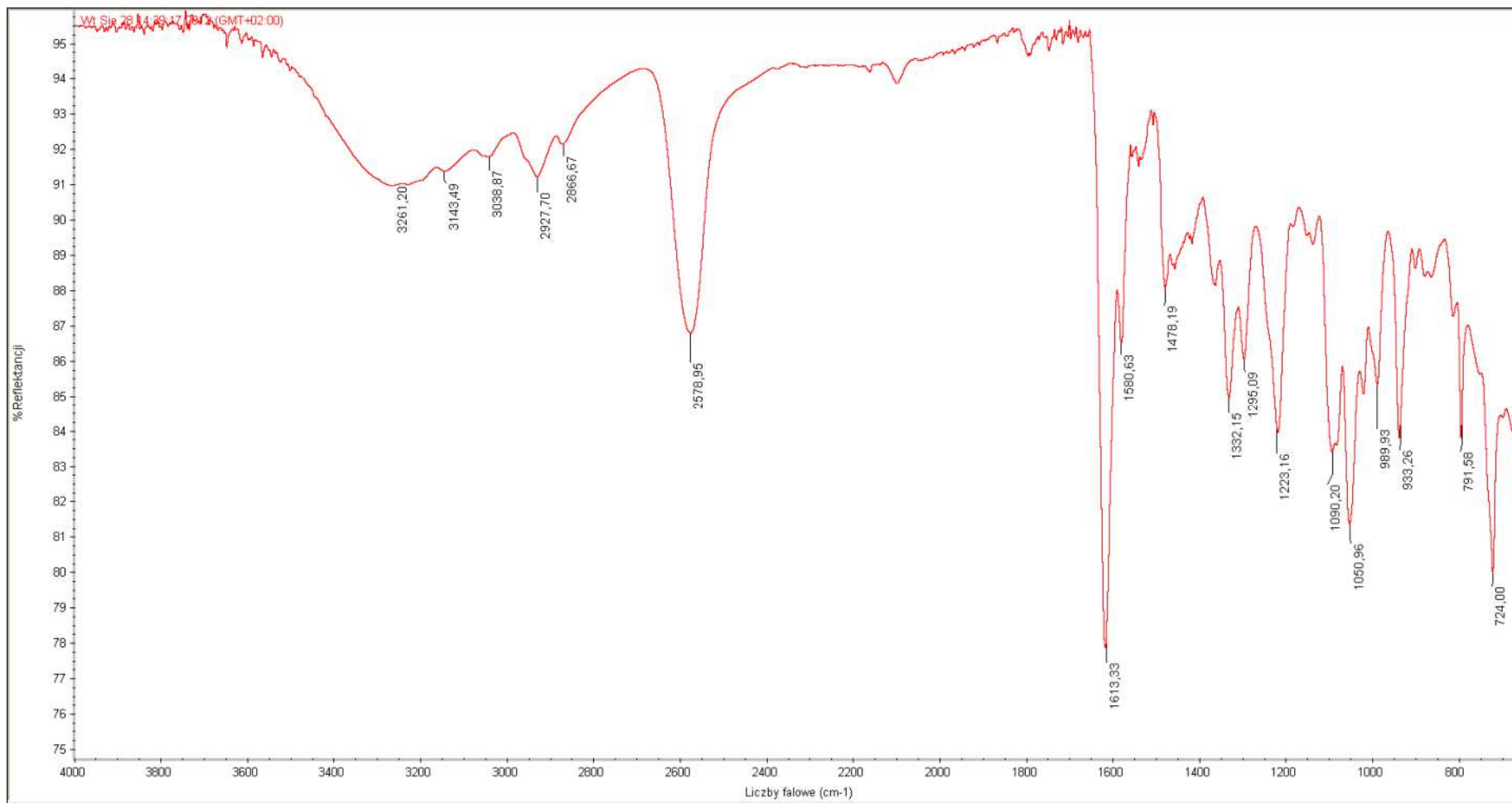


Figure S57. IR spectrum of compound **24**.

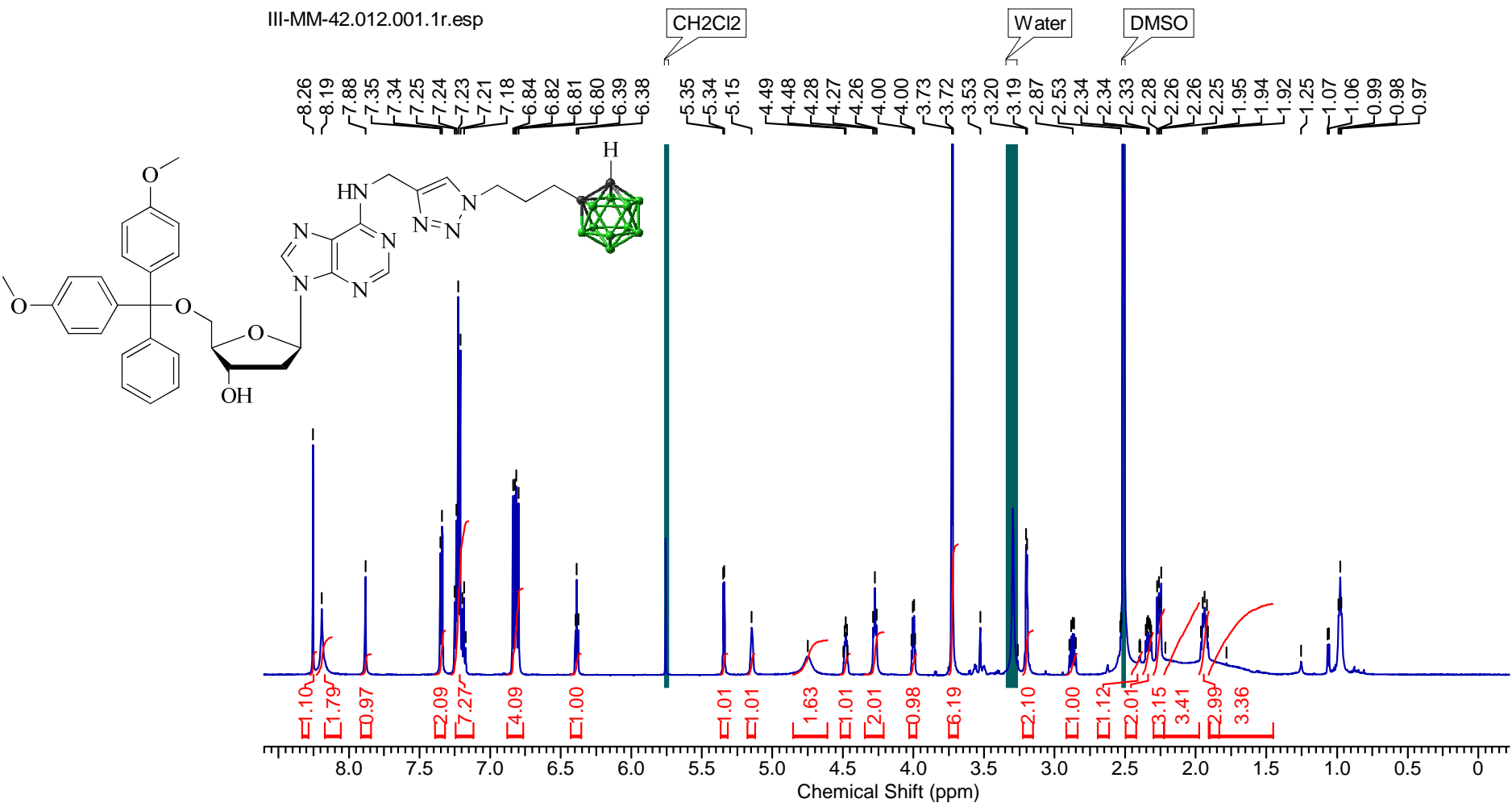


Figure S59. ¹H NMR spectrum of compound 25.

III-MM-42.010.001.1r.esp

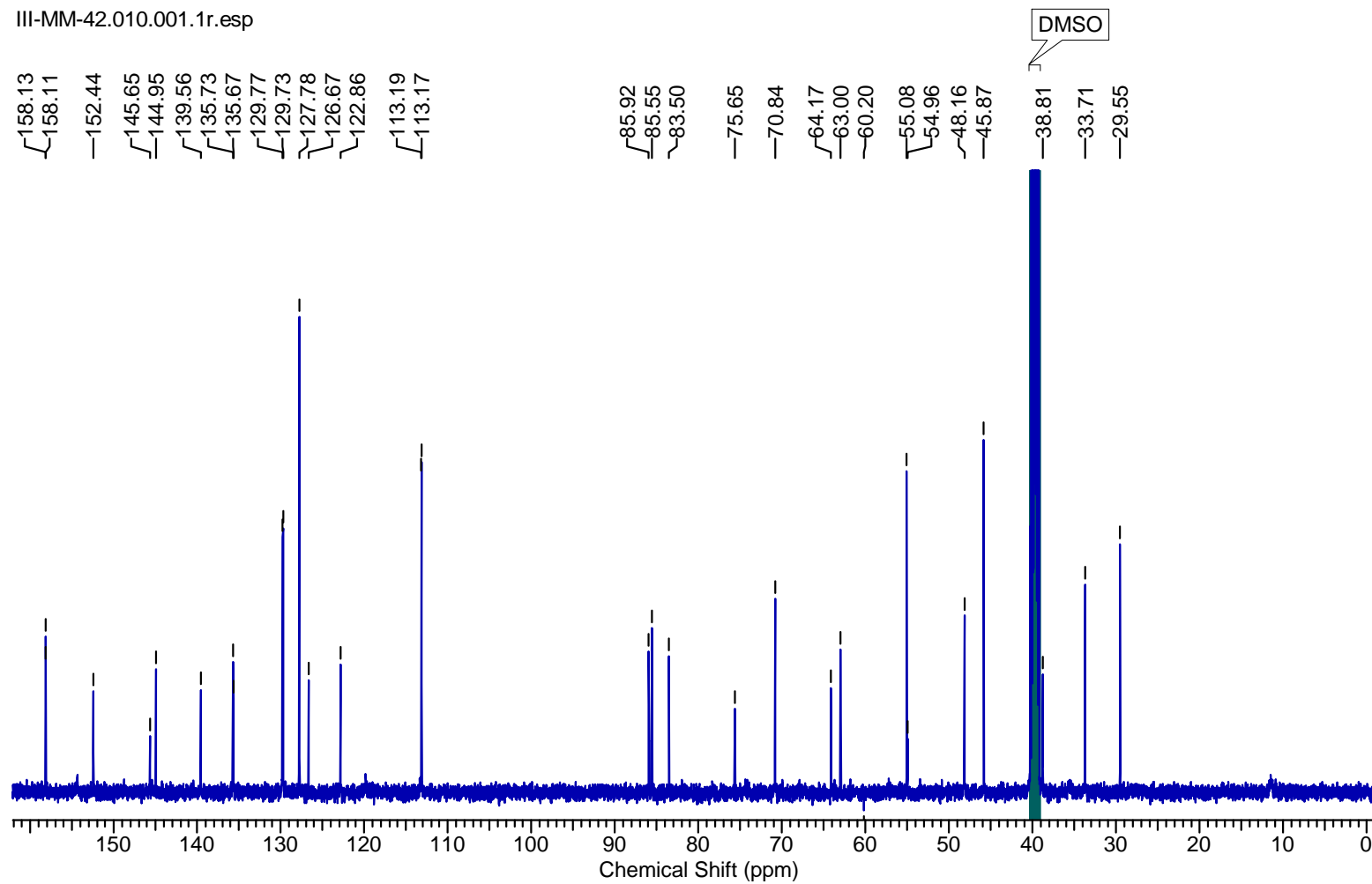


Figure S60. ^{13}C NMR spectrum of compound 25.

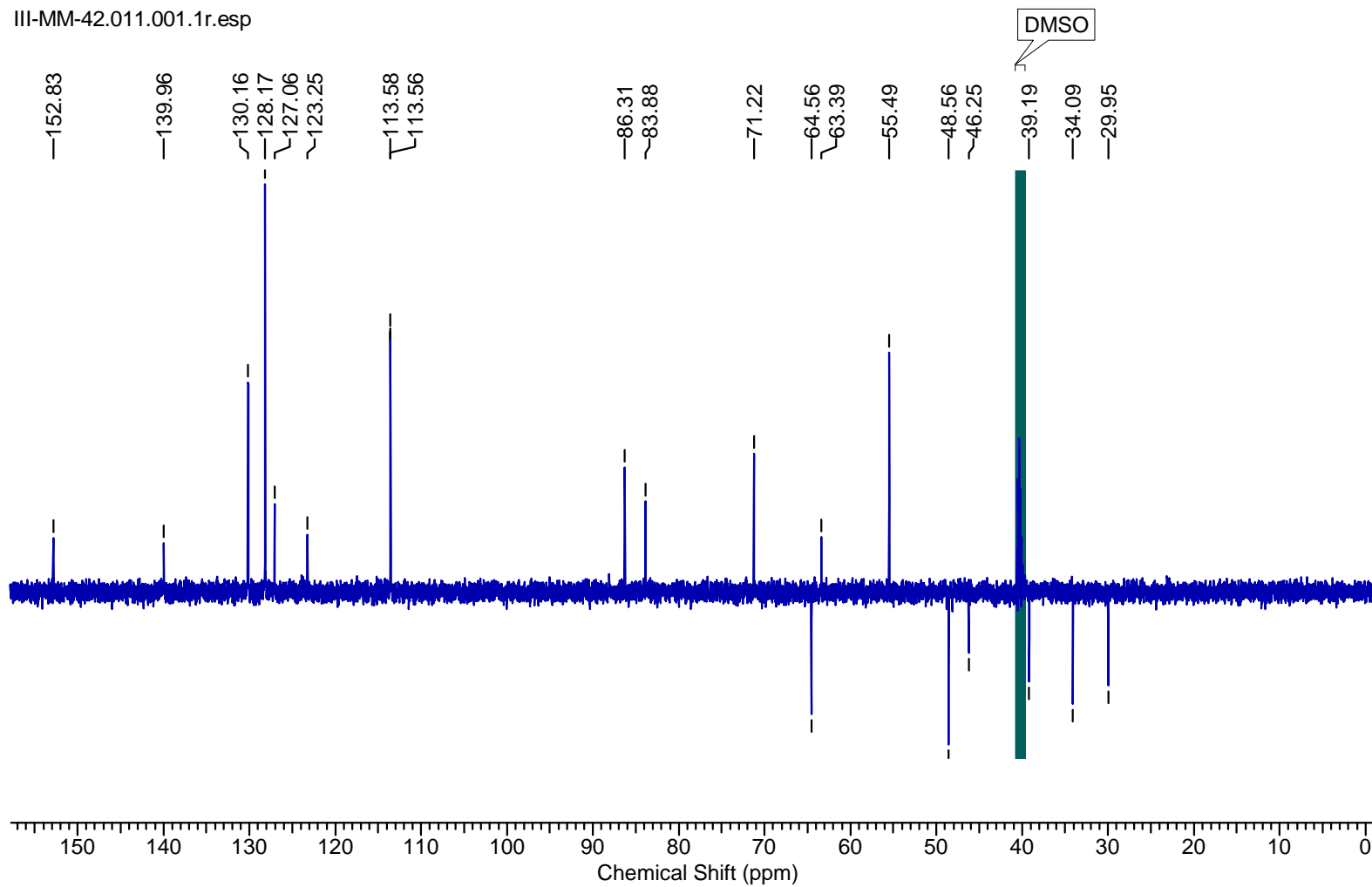


Figure S61. DEPT-135 spectrum of compound **25**.

III-MM-42.003.001.1r.esp

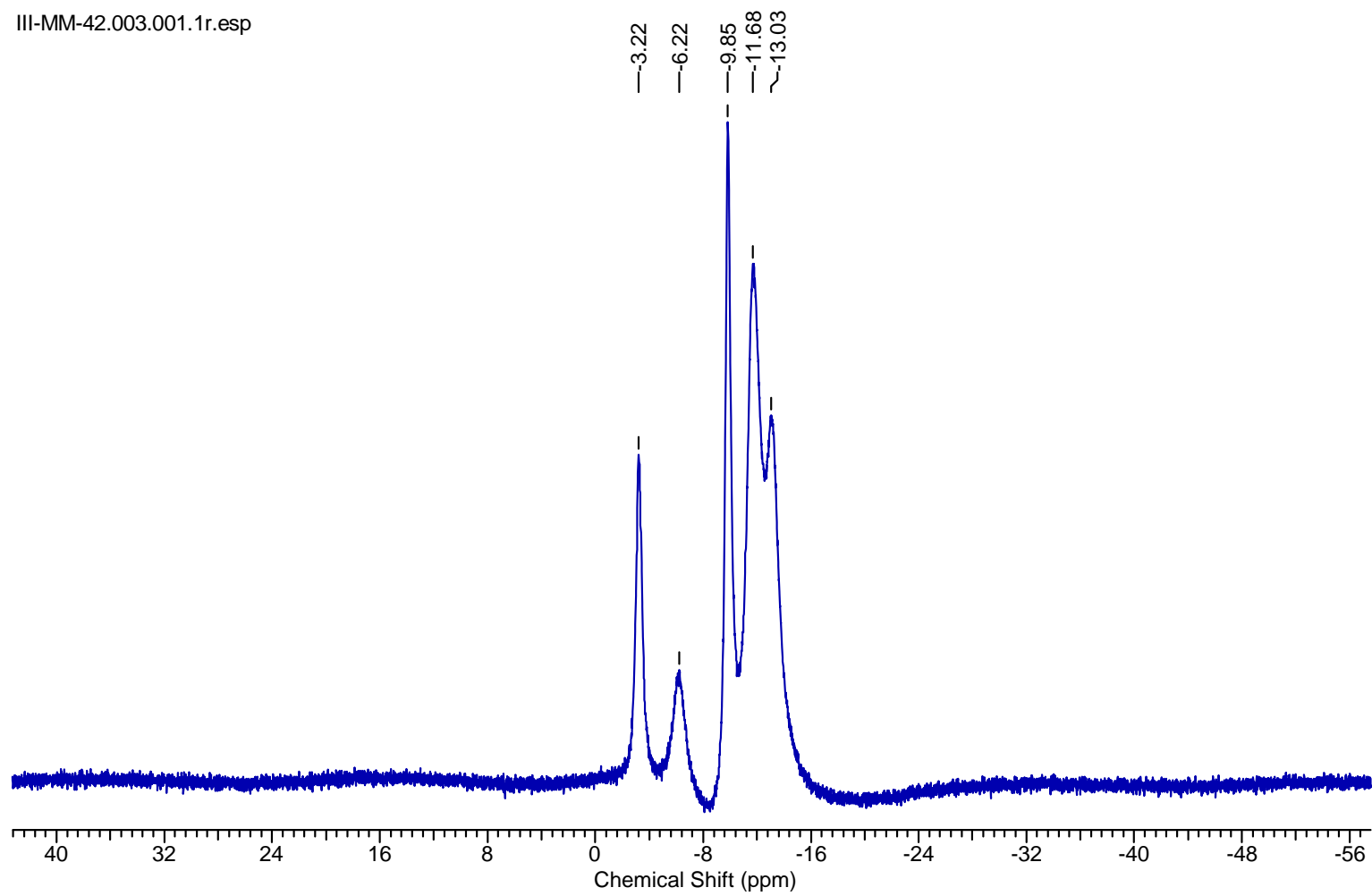


Figure S62. $^{11}\text{B}\{^1\text{H BB}\}$ NMR spectrum of compound **25**.

III-MM-42.004.001.1r.esp

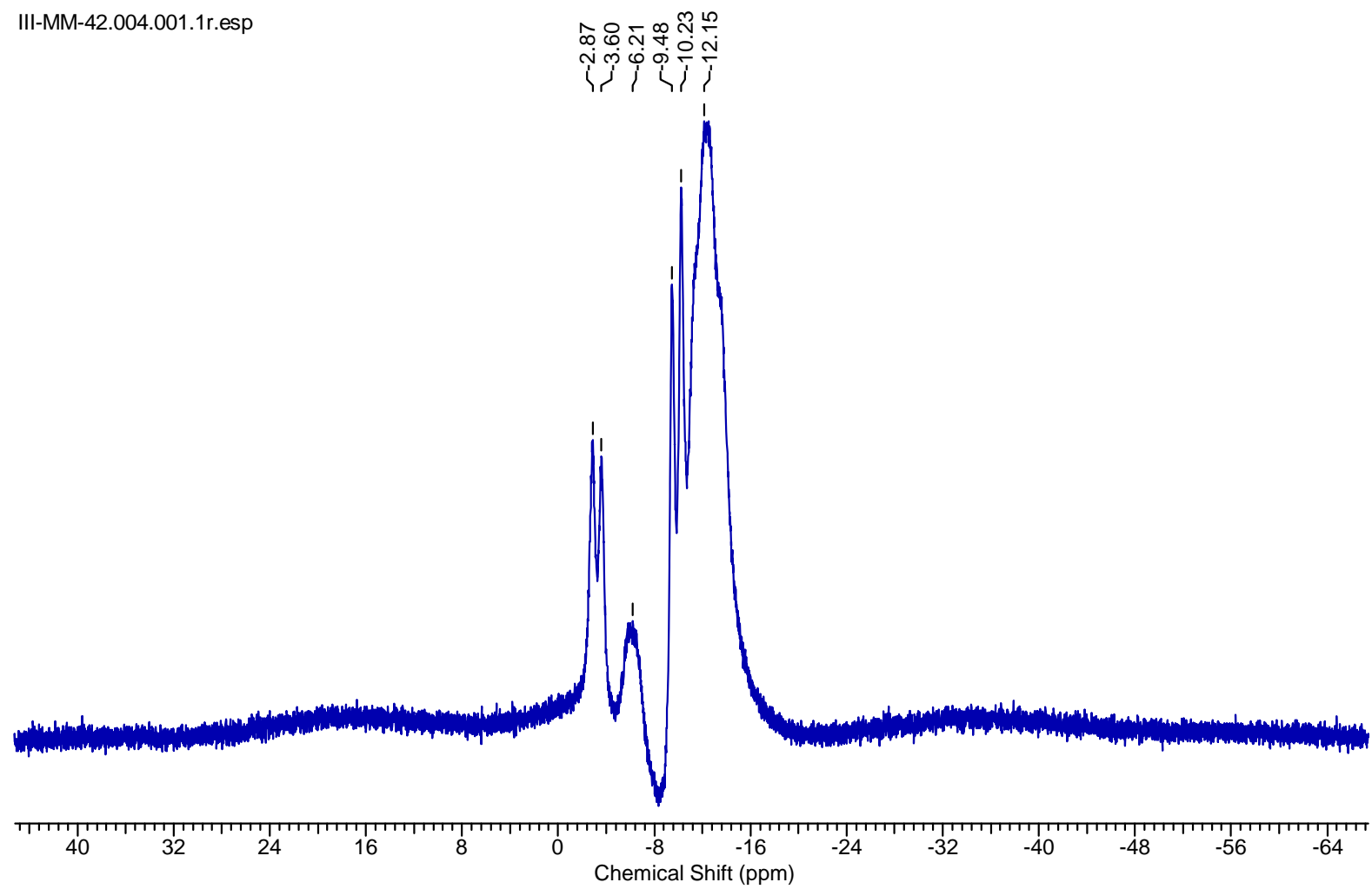


Figure S63. ^{11}B NMR spectrum of compound **25**.

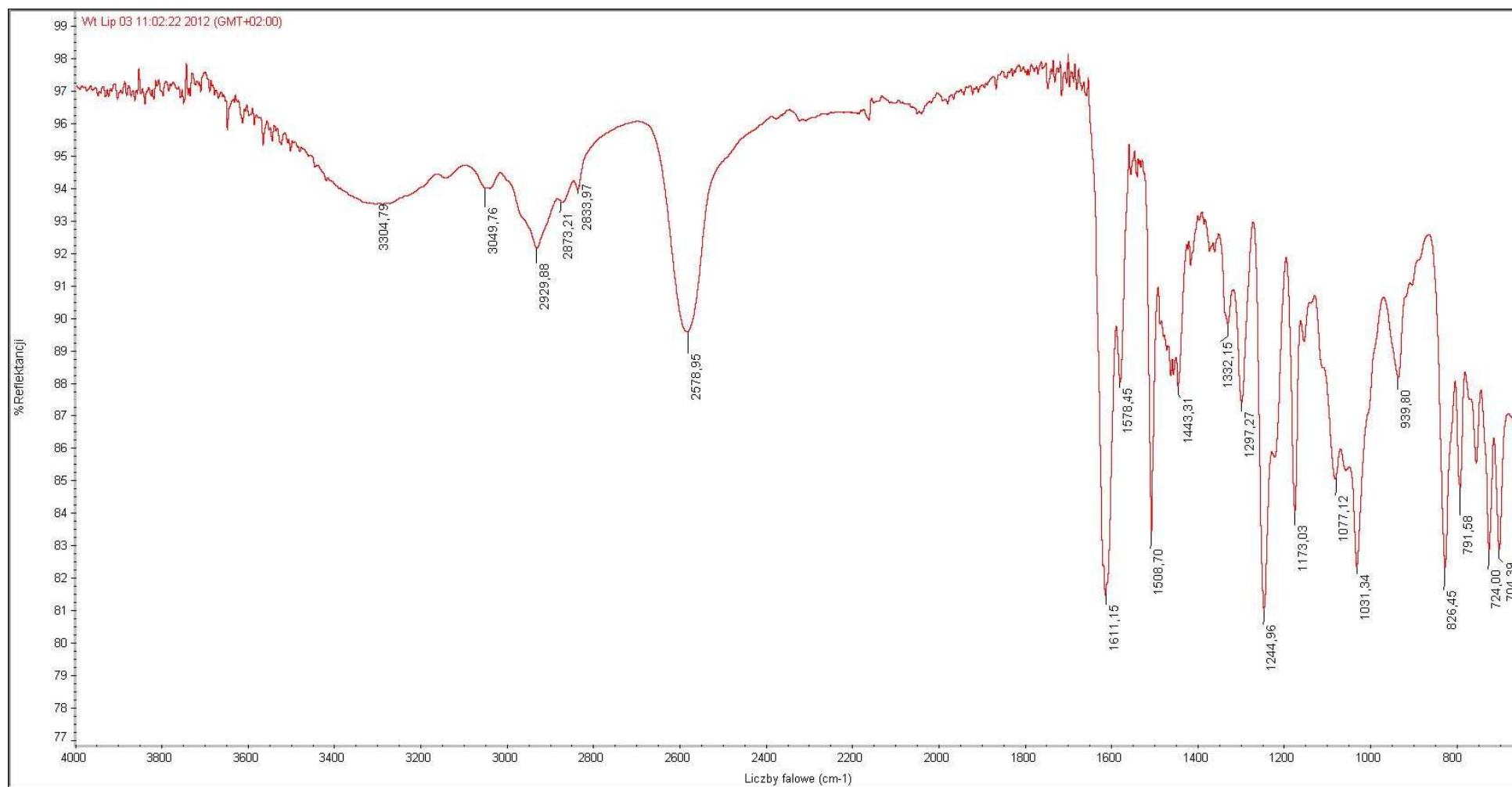
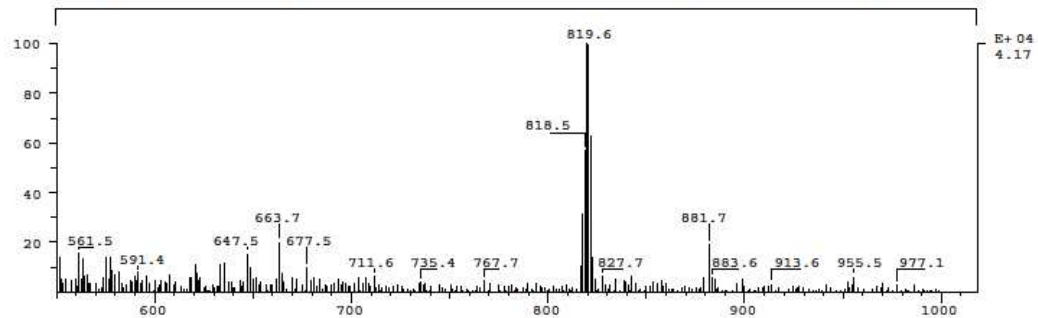
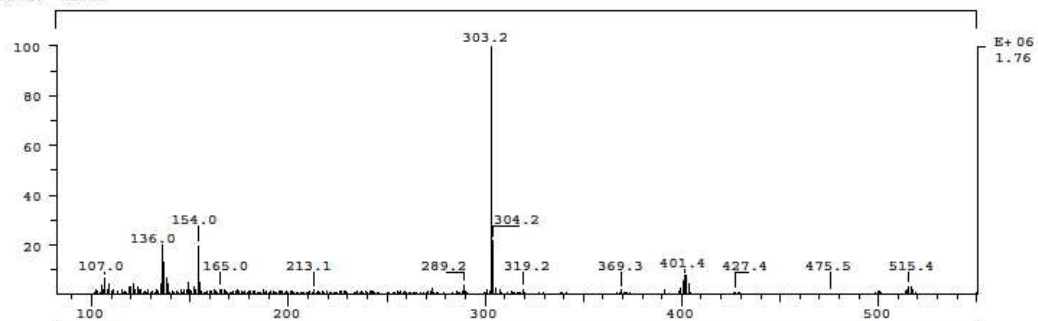


Figure S64. IR spectrum of compound **25**.

SPEC: ax6631bm 27-Jun-12 REG : 00:16.4 #9
 Samp: I11-MM-42 Start : 14:20:39 10
 Comm: LSI, Cs+ 13 keV, nba
 Mode: FAB +VE +LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ed Client: IBM A.Olejniczak Inlet :
 Base: 303.2 Inten : 1755645 Masses: 100 > 1000
 Norm: 303.2 RIC : 10029367 #peaks: 759
 Peak: 1000.00 mmu
 Data: +1>10



SPEC: ax6631bm_a 27-Jun-12 REG : 00:16.4 #9
 Samp: I11-MM-42 Start : 14:24:38 10
 Comm: LSI, Cs+ 13 keV, nba
 Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ed Client: IBM A.Olejniczak Inlet :
 Base: 152.9 Inten : 36550 Masses: 100 > 1000
 Norm: 152.9 RIC : 408968 #peaks: 366
 Peak: 1000.00 mmu
 Data: +1>10

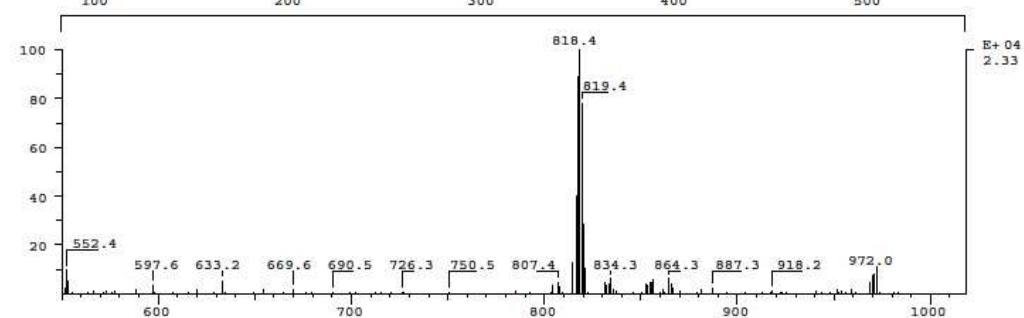
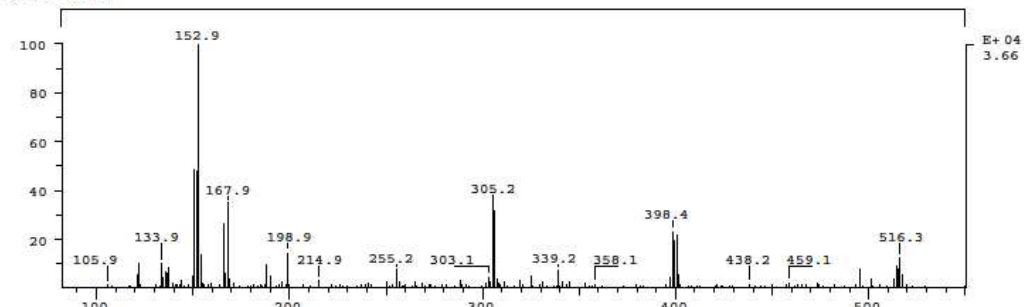


Figure S65. MS spectra of compound 25.

III-MM-48.010.001.1r.esp

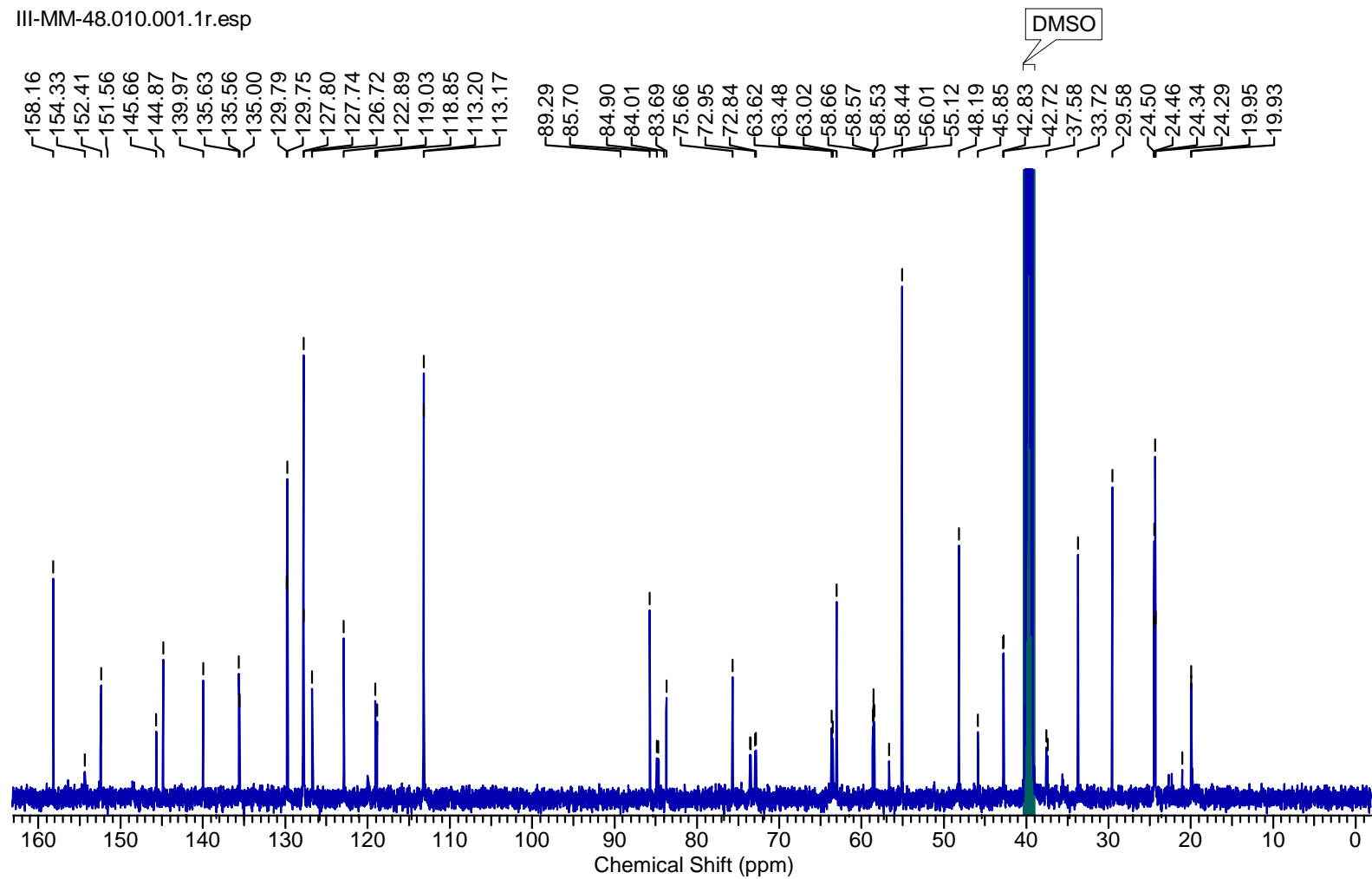


Figure S67. ^{13}C NMR spectrum of compound **31**.

III-MM-48.011.001.1r.esp

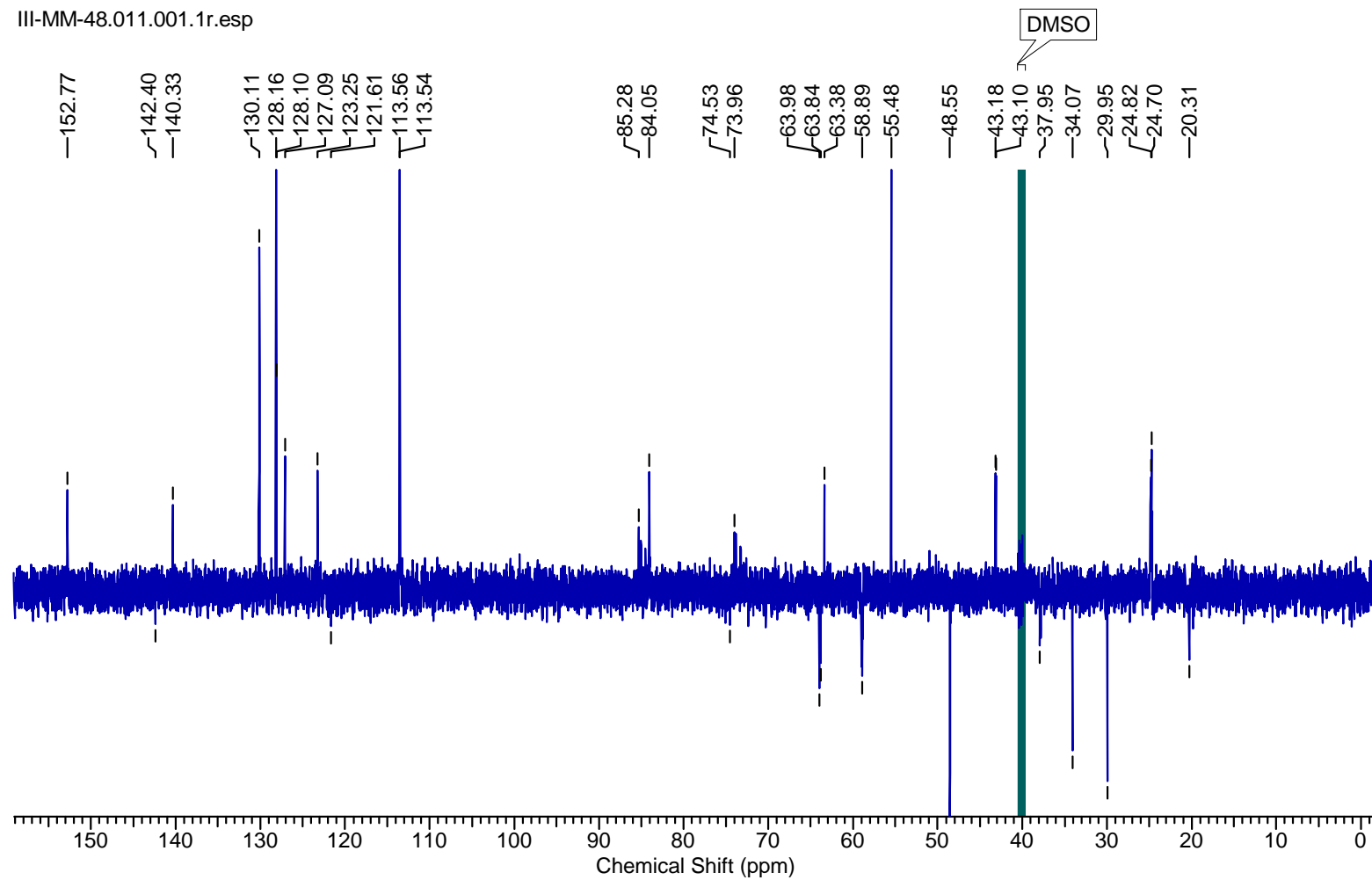


Figure S68. DEPT-135 spectrum of compound **31**.

III-MM-48.003.001.1r.esp

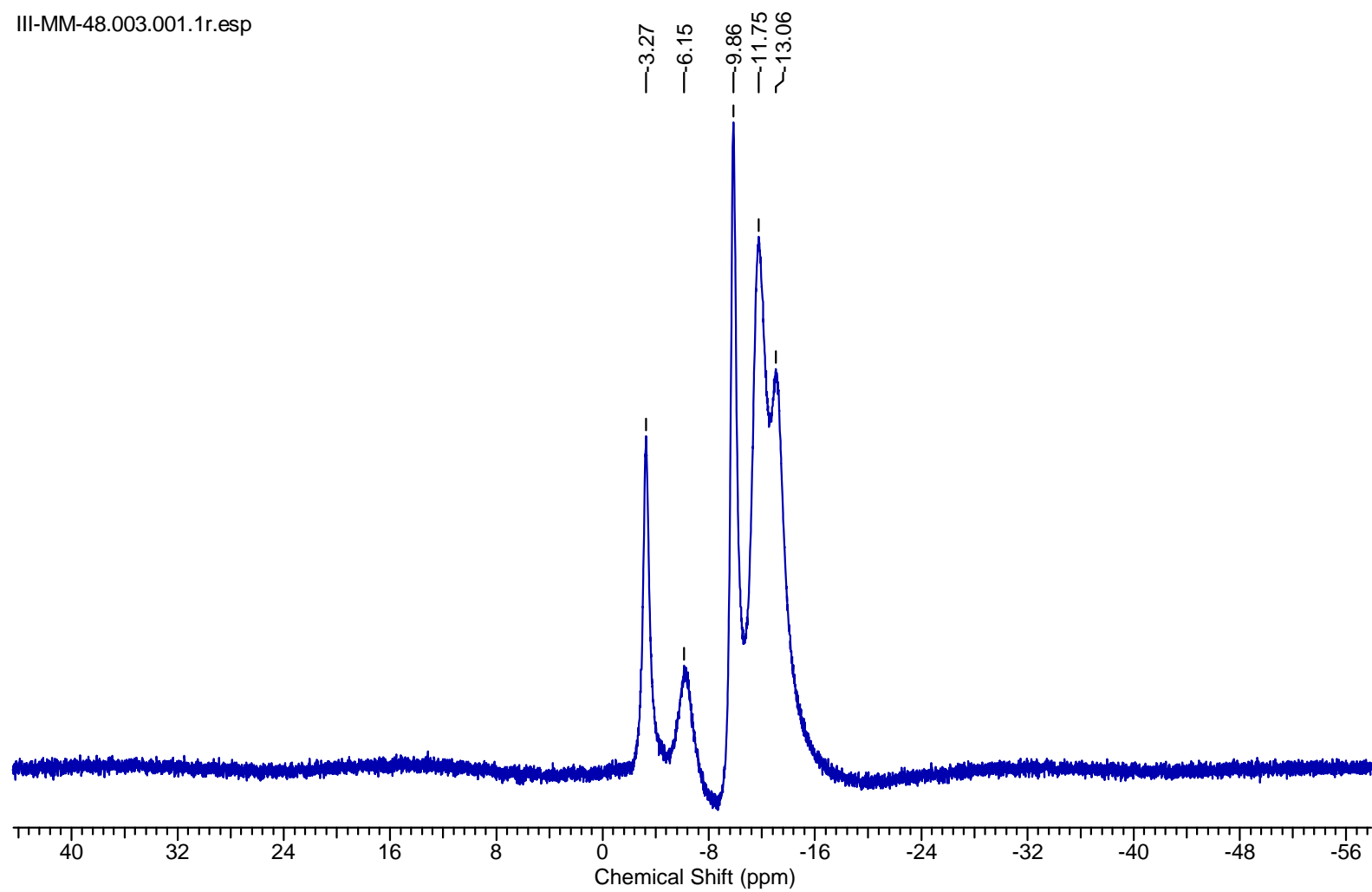


Figure S69. $^{11}\text{B}\{^1\text{H BB}\}$ NMR spectrum of compound **31**.

III-MM-48.004.001.1r.esp

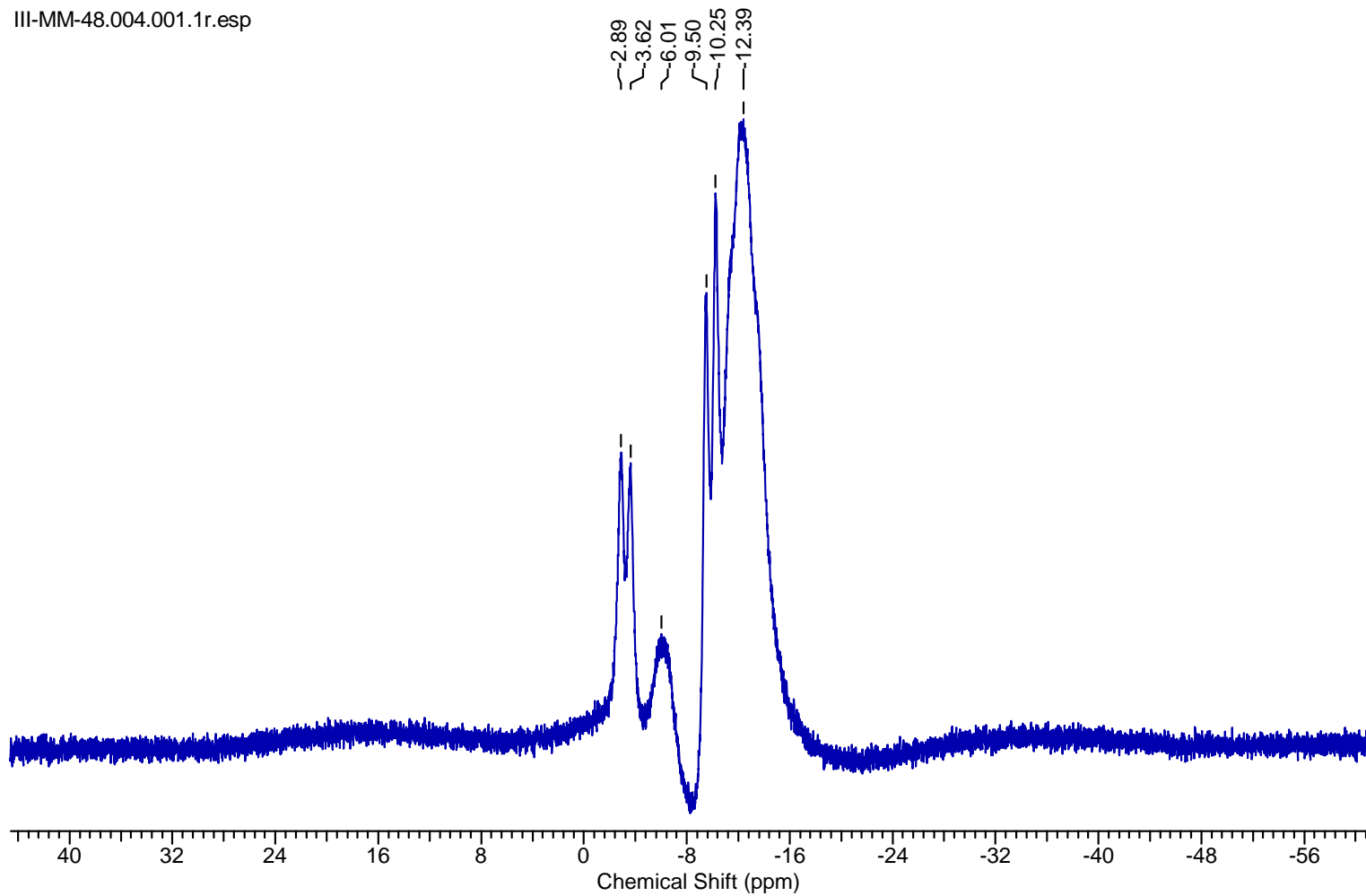


Figure S70. ^{11}B NMR spectrum of compound **31**.

III-MM-48.017.001.1r.esp

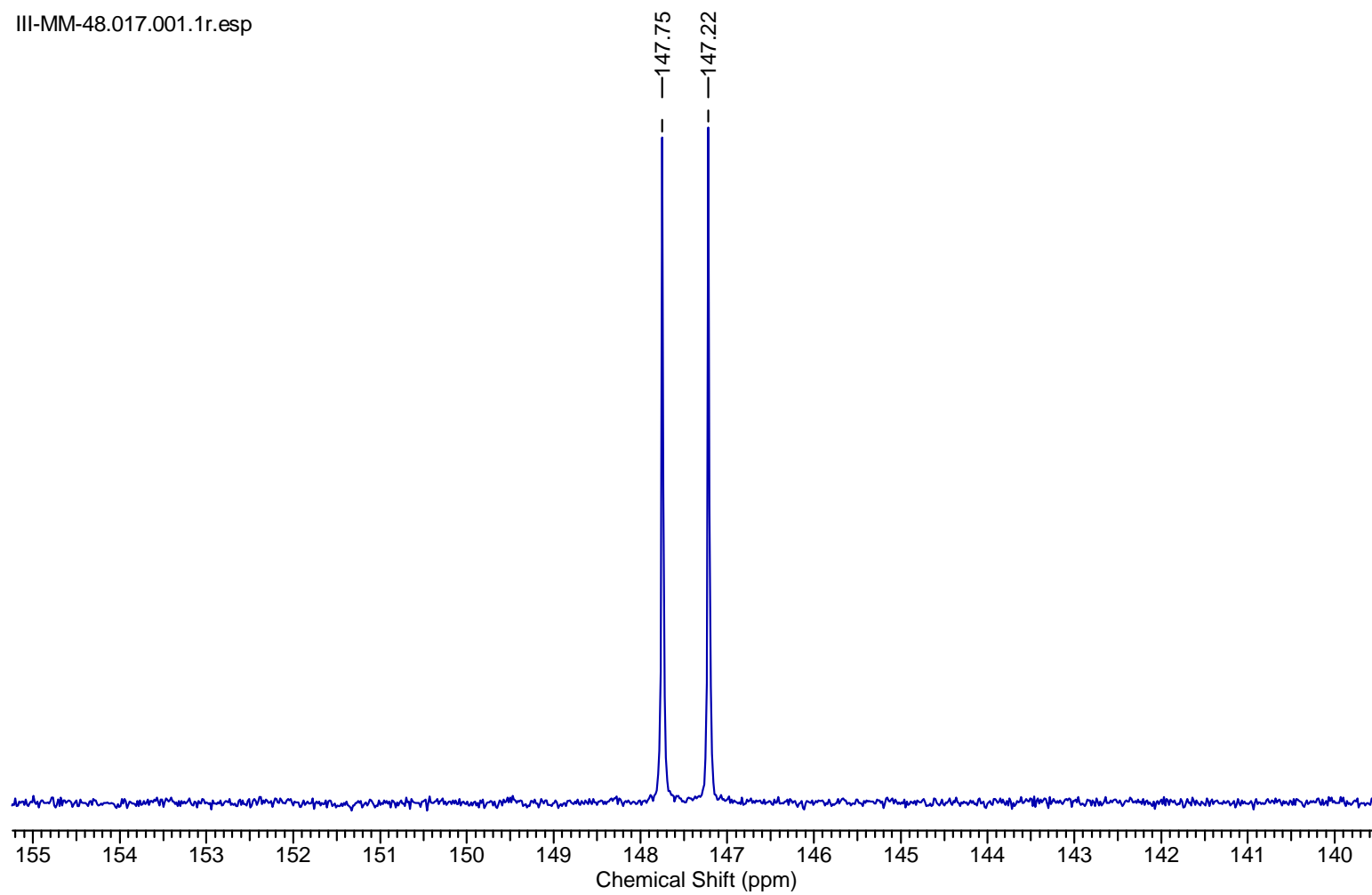


Figure S71. ^{31}P NMR spectrum of compound **31**.

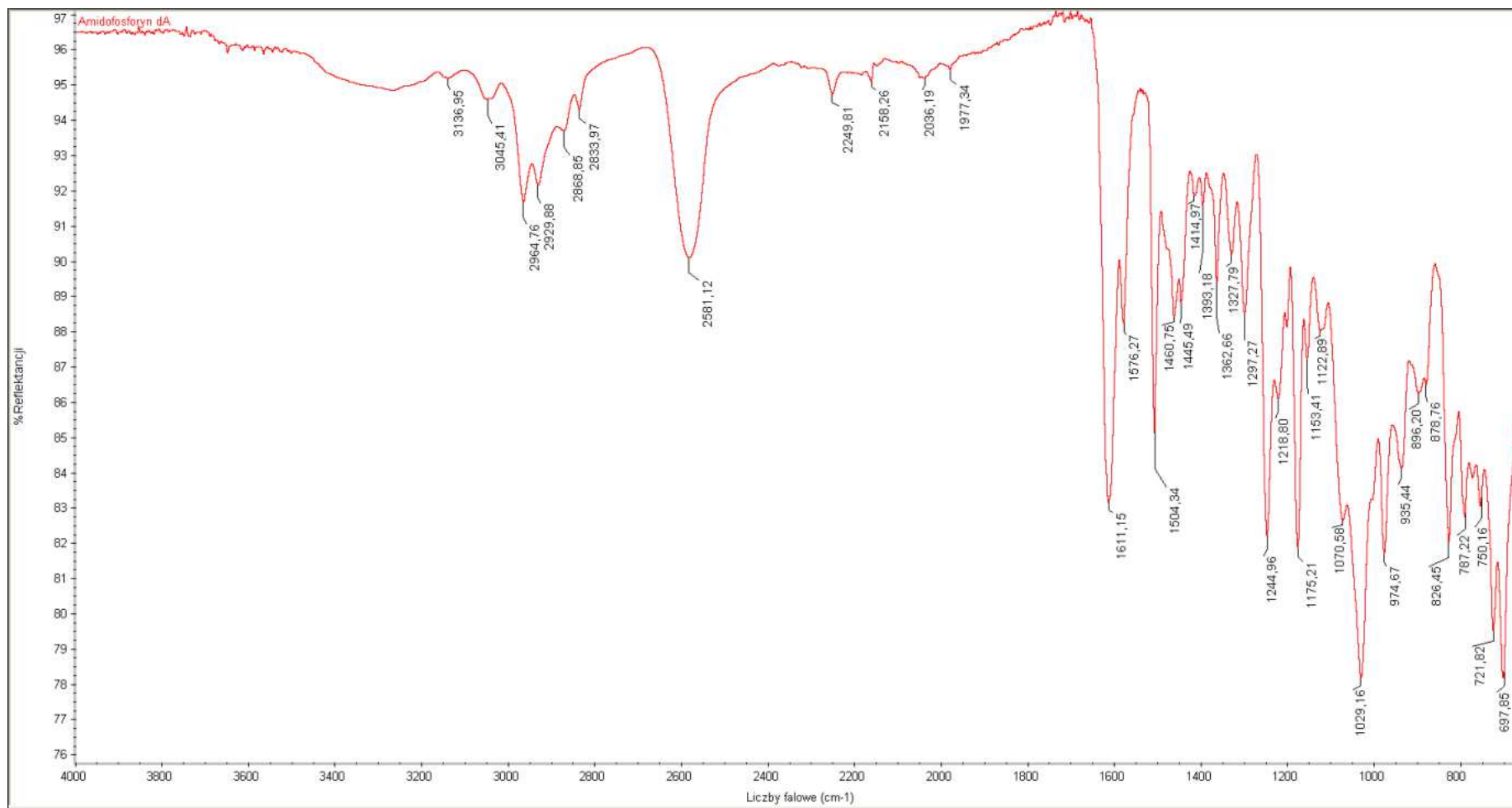


Figure S72. IR spectrum of compound 31.

SPEC: ax7461bm a 12-Jul-12 REG : 00:16.8 #9
 Samp: I11-MM-48 Start : 09:50:51 10
 Comm: LSI, Cs+ 13 keV, nba
 Mode: FAB +VE +LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ed Client: IBM A.Olejniczak Inlet :
 Base: 303.2 Inten : 2209754 Masses: 100 > 1117
 Norm: 303.2 RIC : 7394358 #peaks: 530
 Peak: 1000.00 mmu
 Data: +1>10

SPEC: ax7461bm 12-Jul-12 REG : 00:16.8 #9
 Samp: I11-MM-48 Start : 09:45:49 10
 Comm: LSI, Cs+ 13 keV, nba
 Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ed Client: IBM A.Olejniczak Inlet :
 Base: 152.9 Inten : 403214 Masses: 100 > 1117
 Norm: 152.9 RIC : 2810976 #peaks: 536
 Peak: 1000.00 mmu
 Data: +1>10

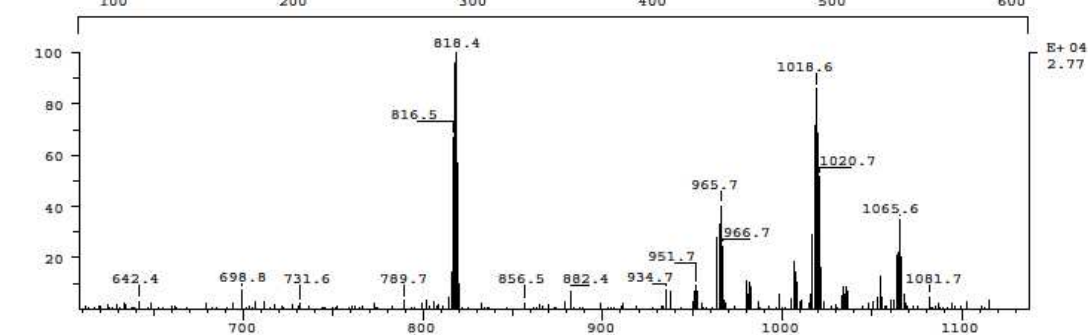
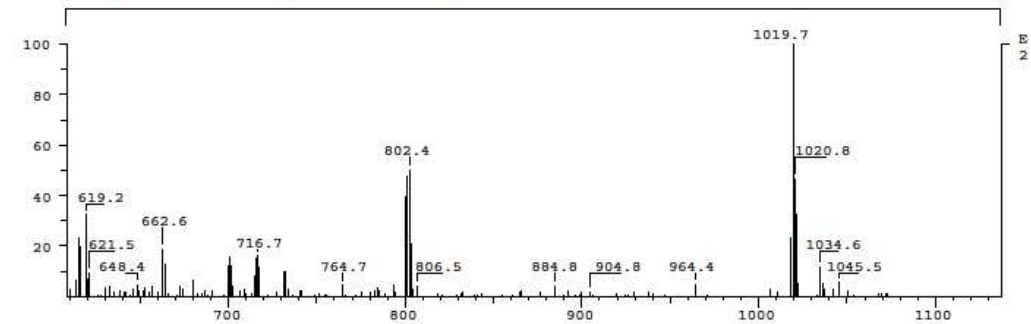
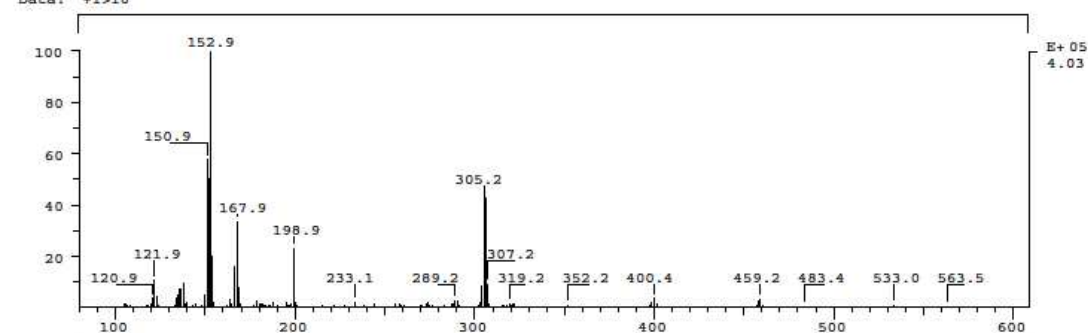
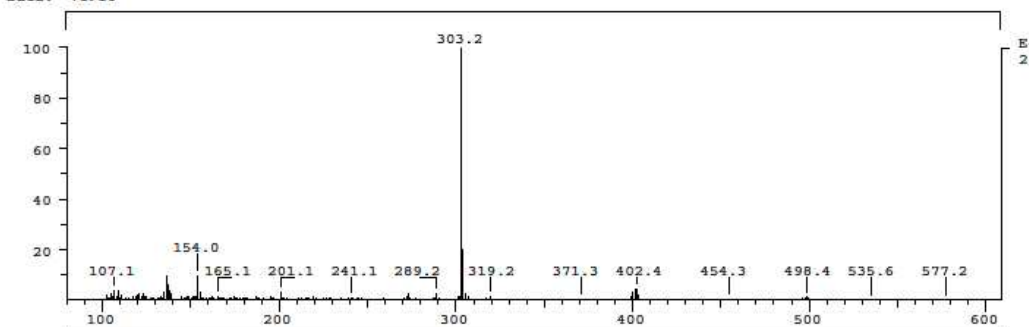


Figure S73. MS-FAB spectra of compound 31.

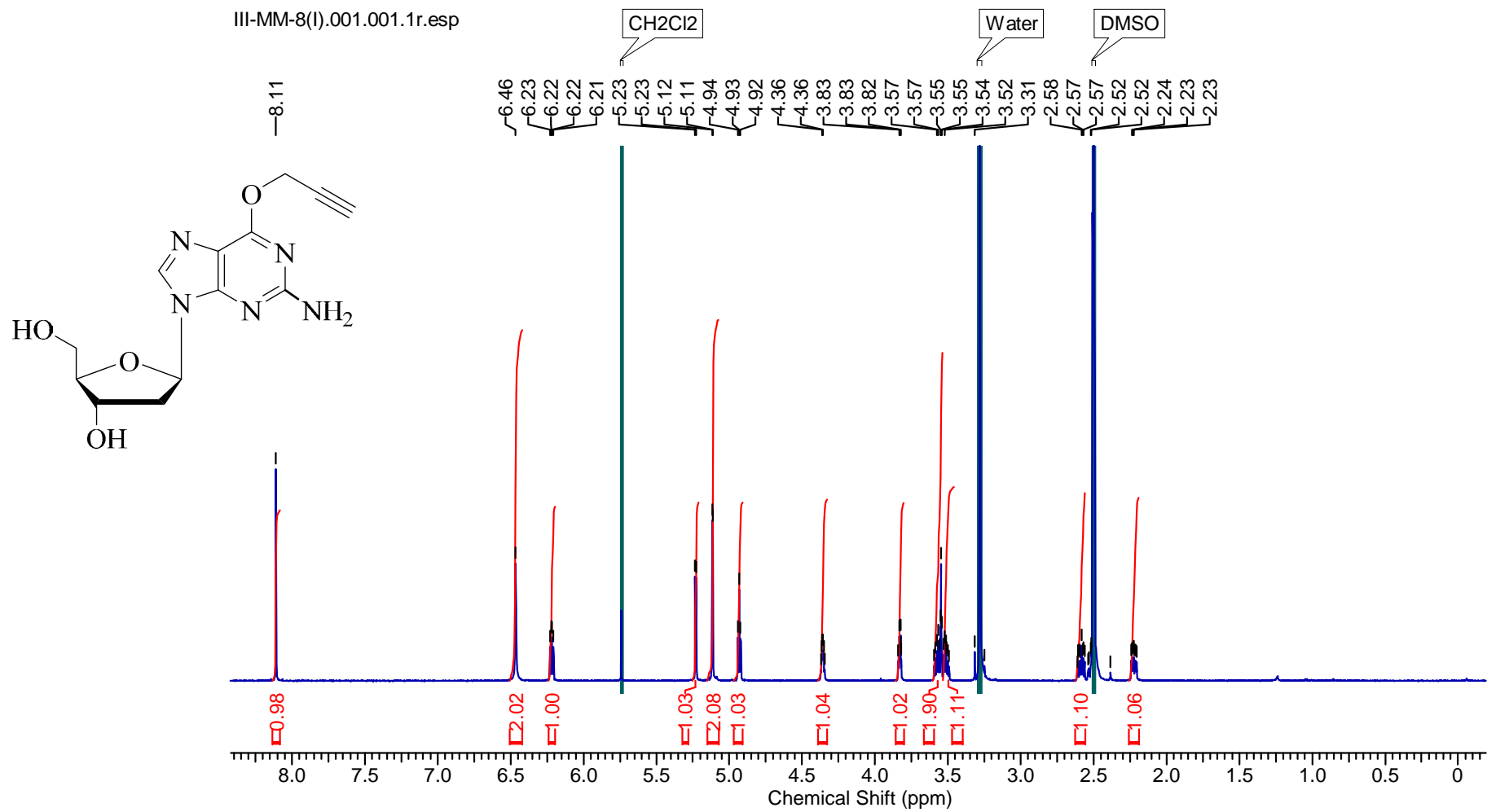


Figure S74. ¹H NMR spectrum of compound 16.

III-MM-52.012.001.1r.esp

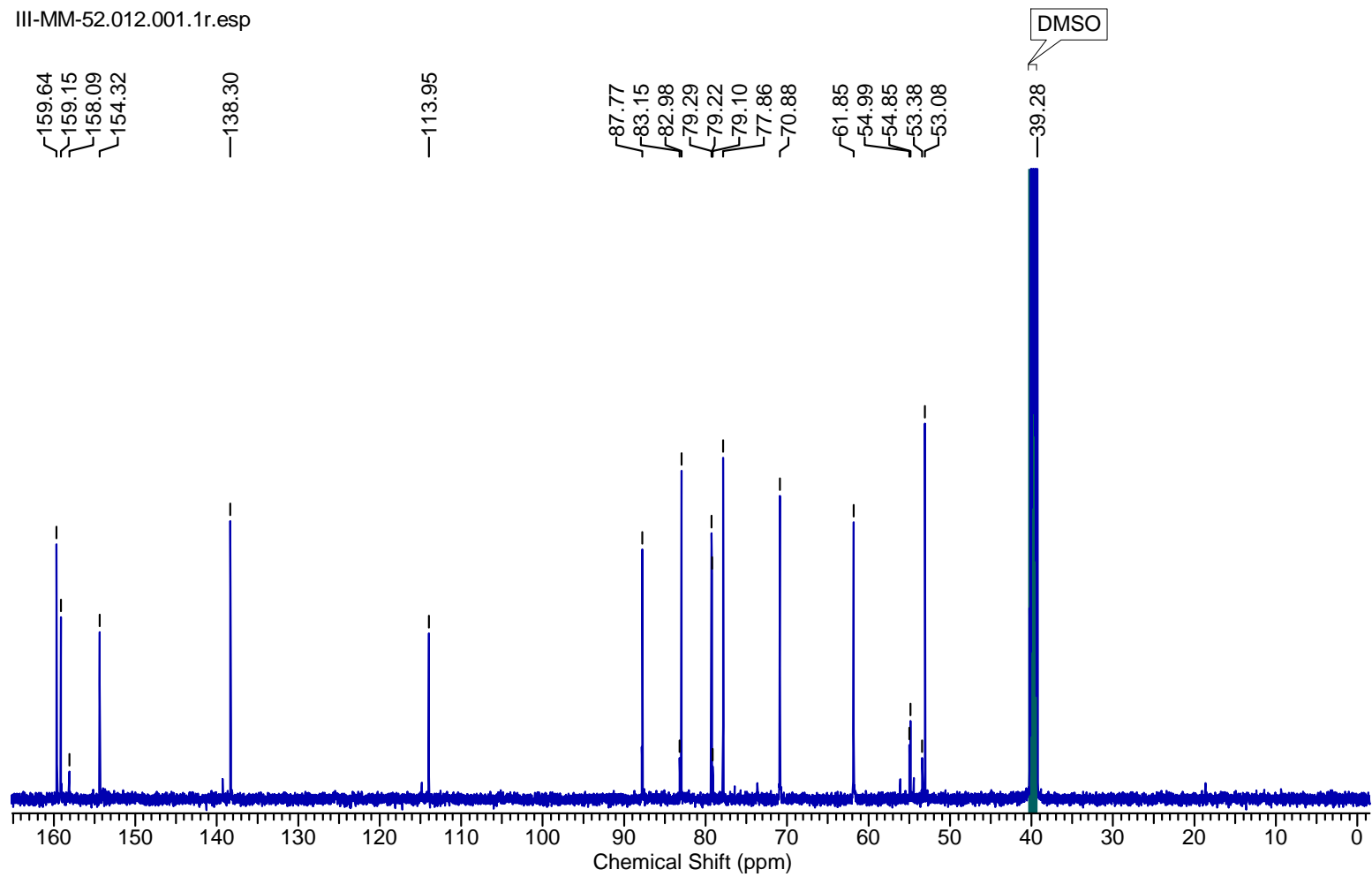


Figure S75. ^{13}C NMR spectrum of compound **16**.

III-MM-52.013.001.1r.esp

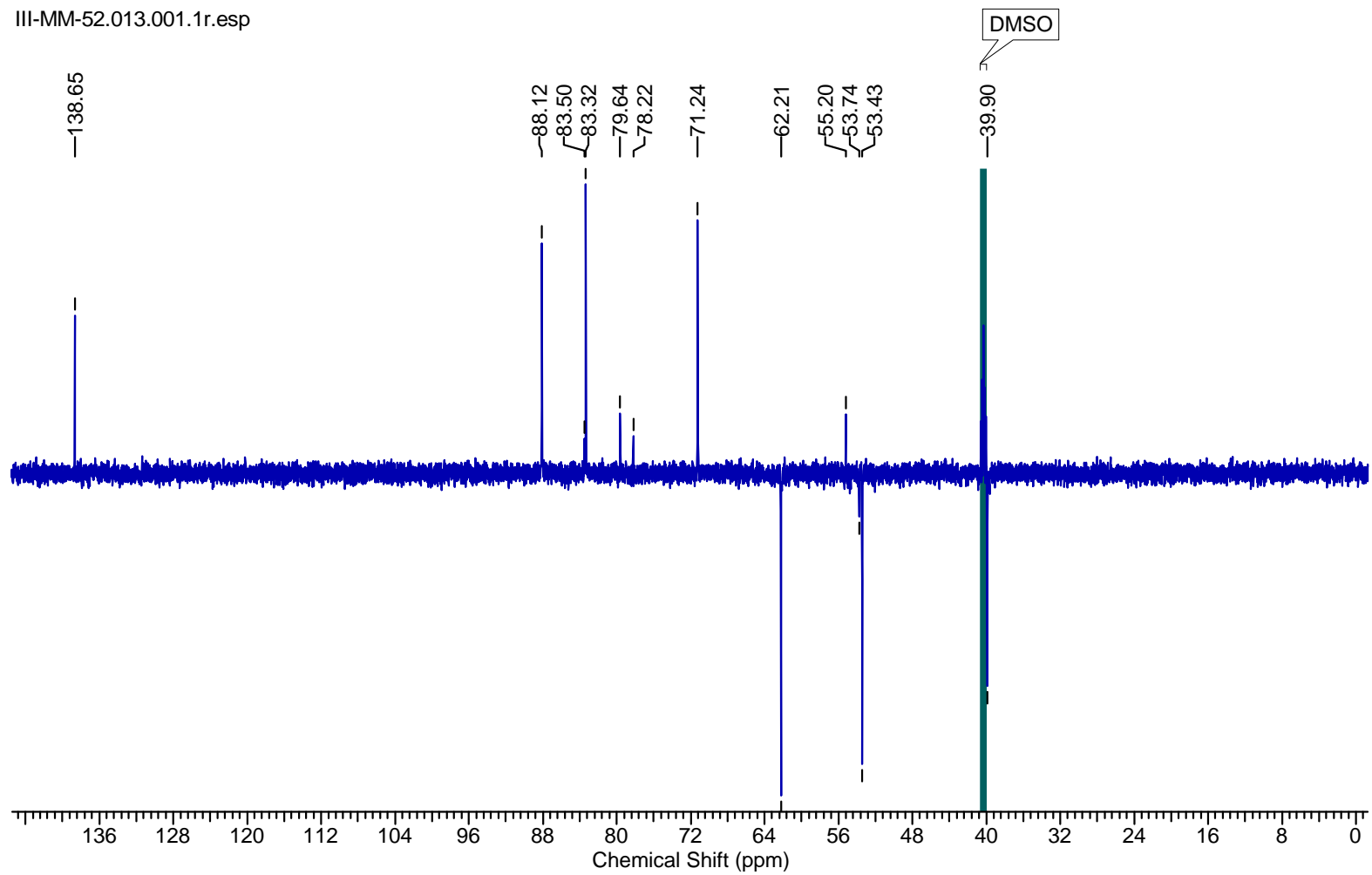


Figure S76. DEPT-135 spectrum of compound **16**.

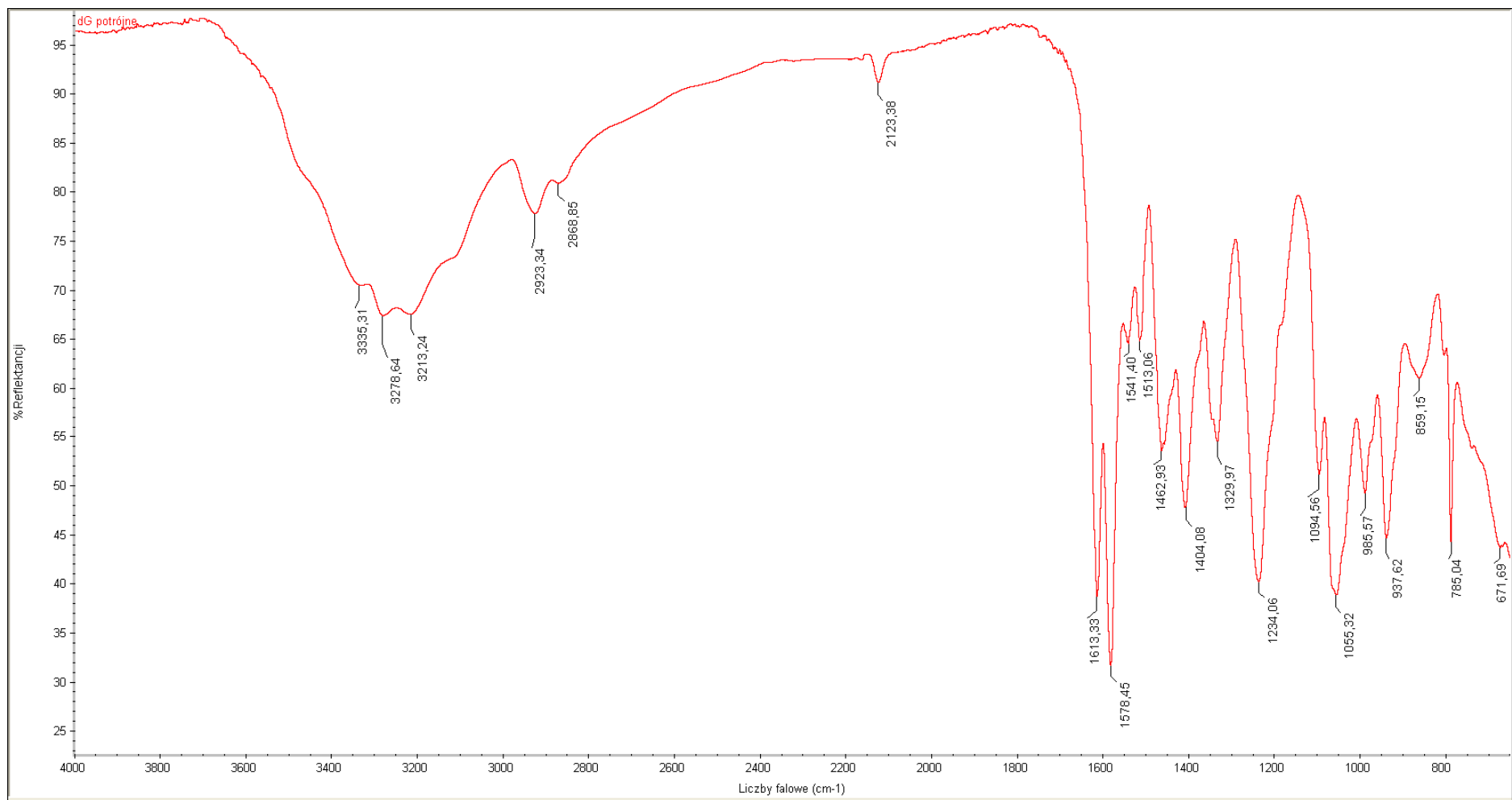


Figure S77. IR spectrum of compound **16**.

SPEC: ax5301bm_a 30-May-12 REG : 00:16.4 #9
 Samp: III-MM-8(I) Start : 14:12:22 10
 Comm: LSI, Cs+ 13 keV, gly
 Mode: FAB +VE +LMR BSCAN (EXP) UP LR NRM Study : MS CBM1M PAN Lodz
 Oper: ed Client: IBM A.Olejniczak Inlet :
 Base: 190.1 Inten : 116696 Masses: 100 > 1000
 Norm: 190.1 RIC : 590540 #peaks: 335
 Peak: 1000.00 mmu
 Data: +1>10

SPEC: ax5301bm_b 30-May-12 REG : 00:16.4 #9
 Samp: III-MM-8(I) Start : 14:17:26 10
 Comm: LSI, Cs+ 13 keV, gly
 Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBM1M PAN Lodz
 Oper: ed Client: IBM A.Olejniczak Inlet :
 Base: 266.2 Inten : 107778 Masses: 100 > 1000
 Norm: 266.2 RIC : 670737 #peaks: 441
 Peak: 1000.00 mmu
 Data: +1>10

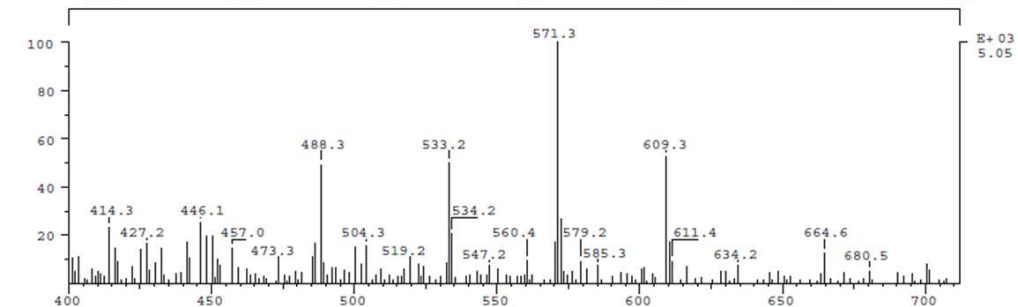
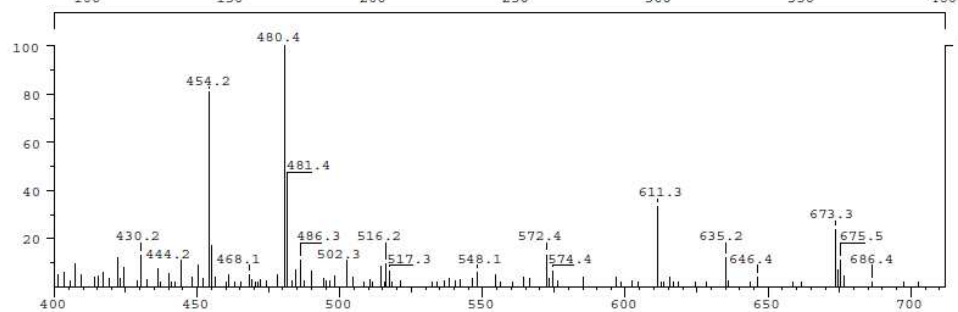
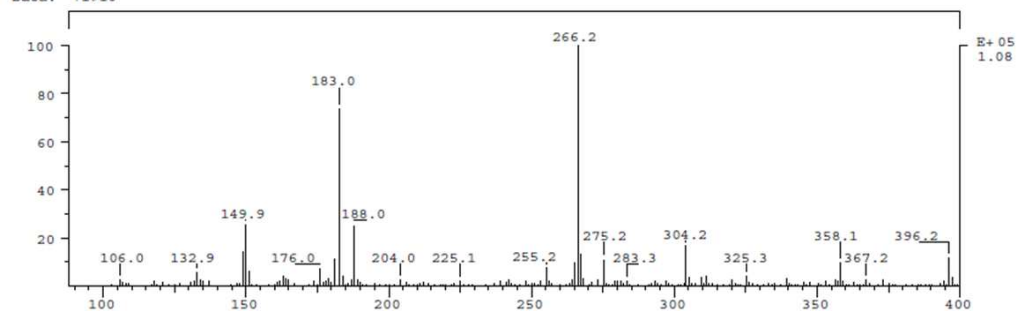
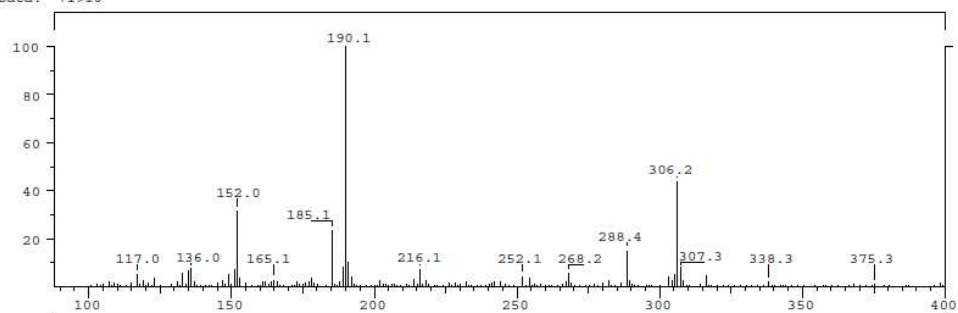


Figure S78. MS-FAB spectra of compound 16.

I-MM-dG-potrojne-trytyl.001.001.1r.esp

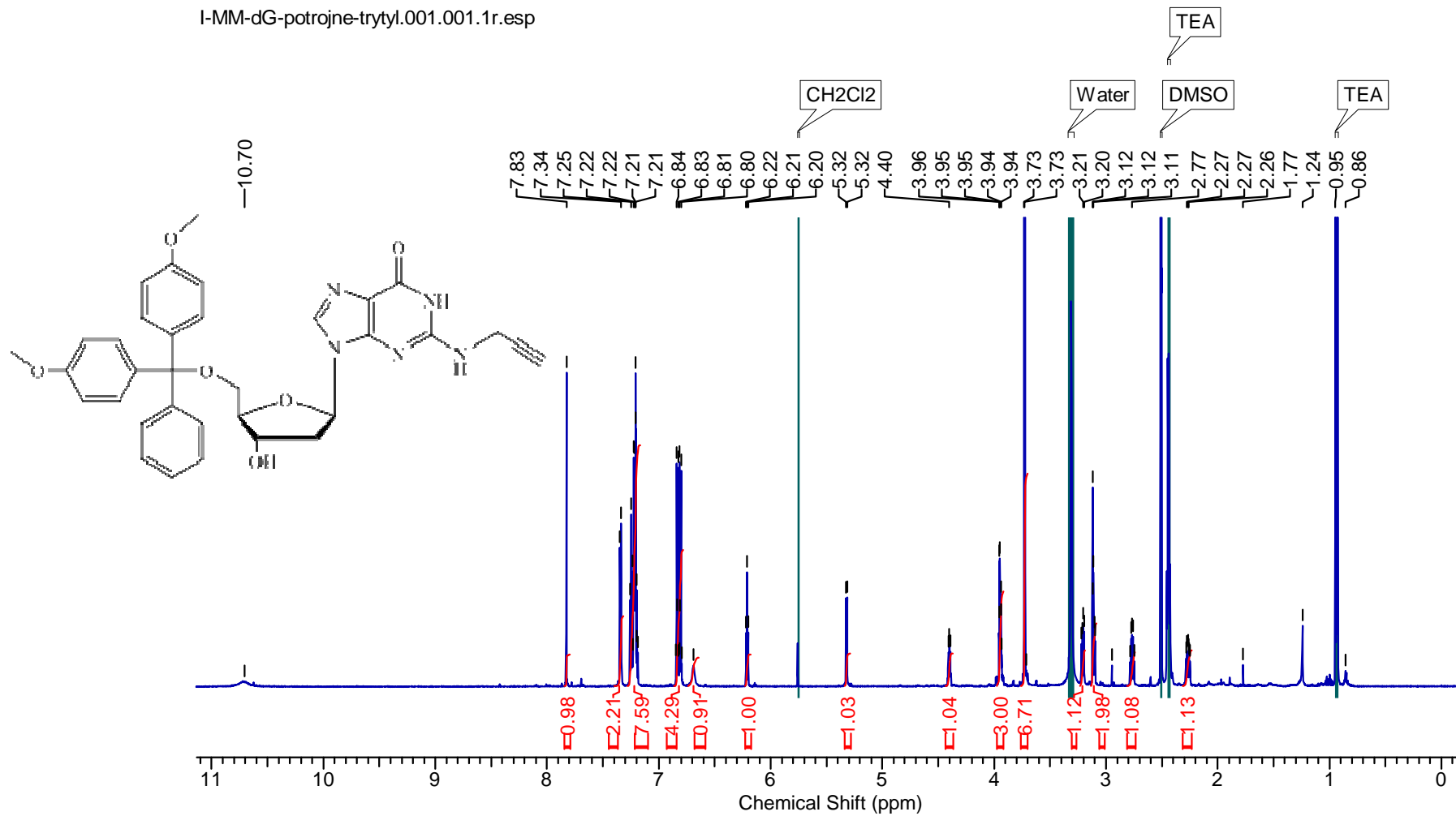


Figure S79. ¹H NMR spectrum of compound 17.

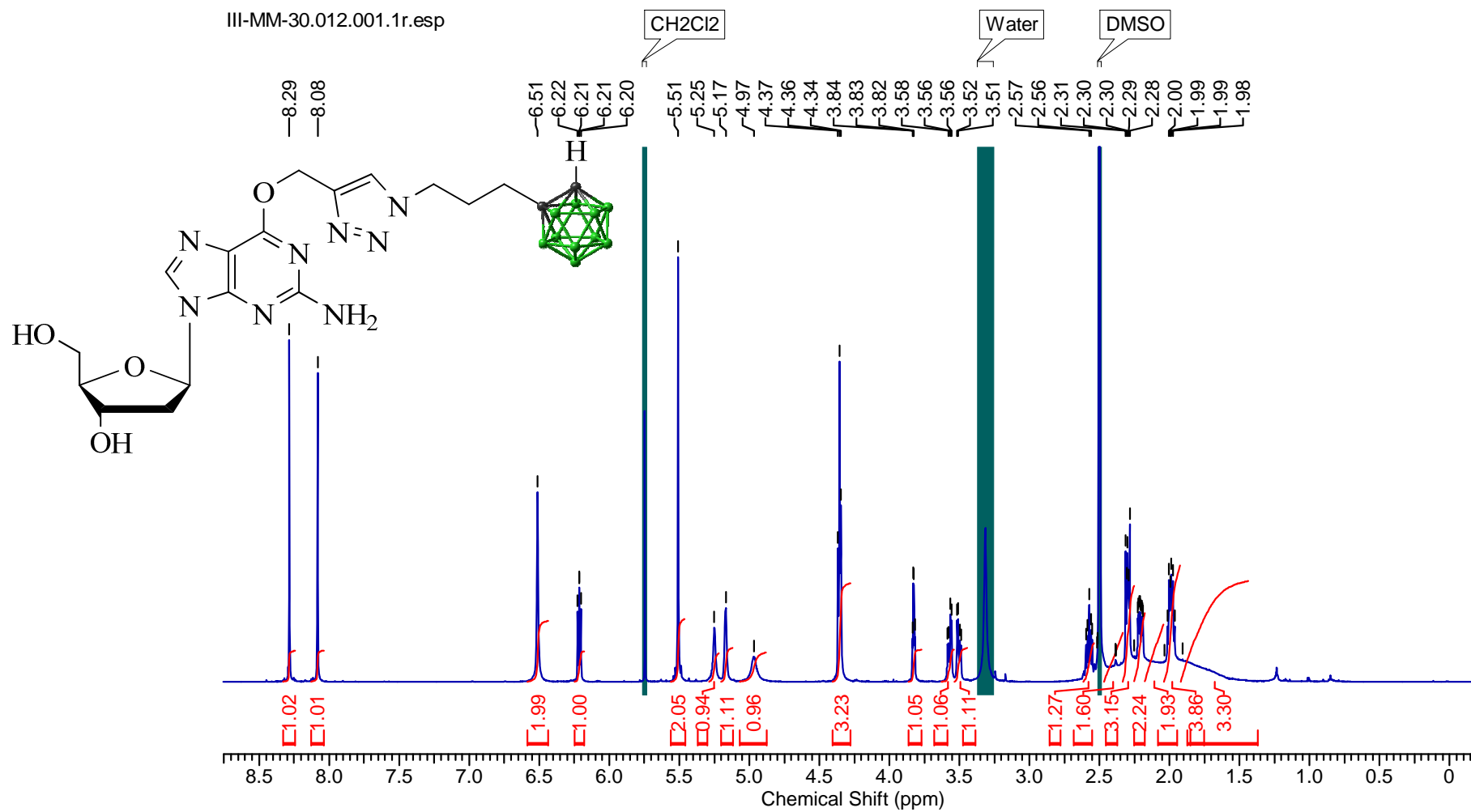


Figure S80. ¹H NMR spectrum of compound 26.

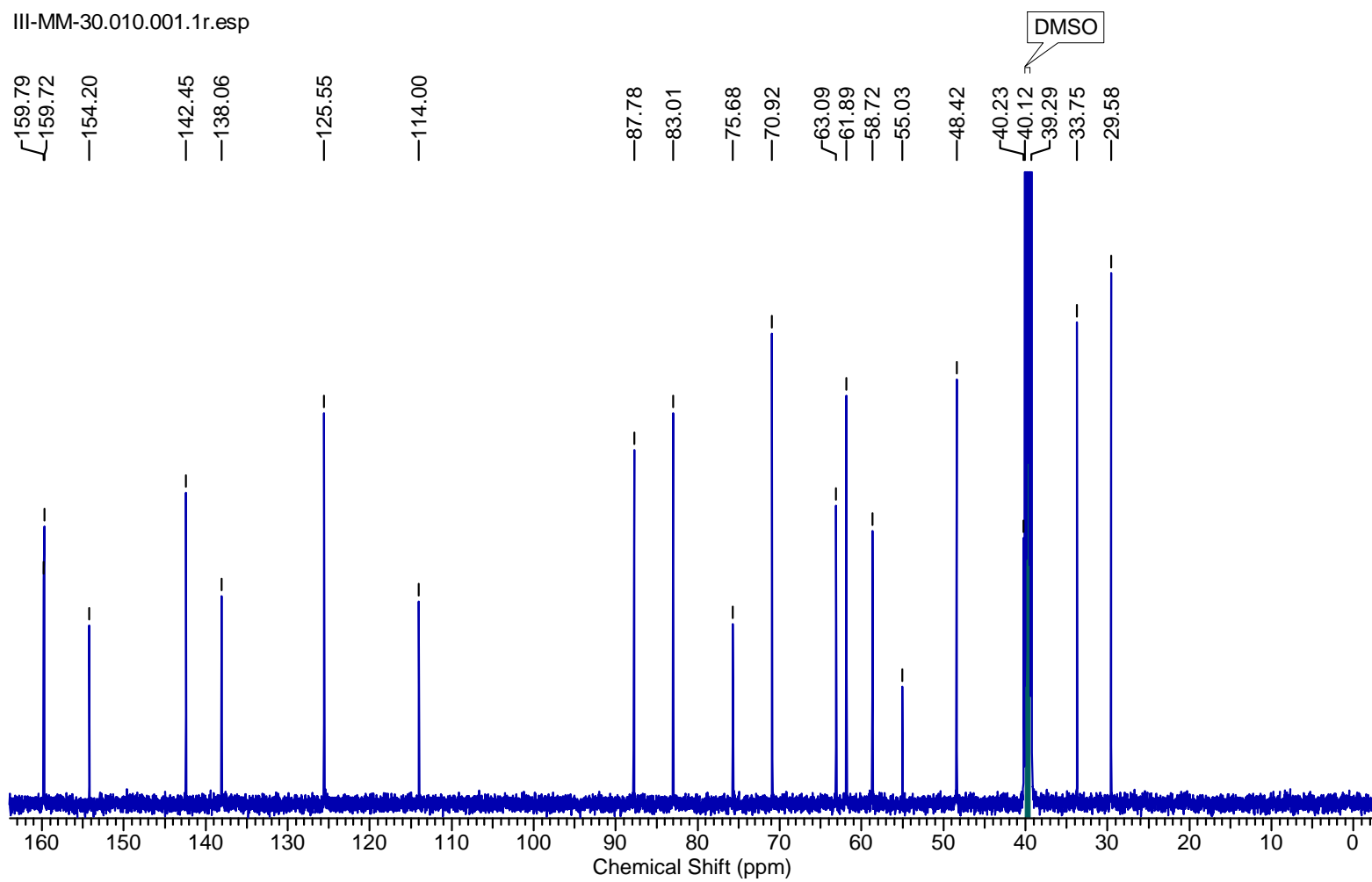


Figure S81. ^{13}C NMR spectrum of compound **26**.

III-MM-30.011.001.1r.esp

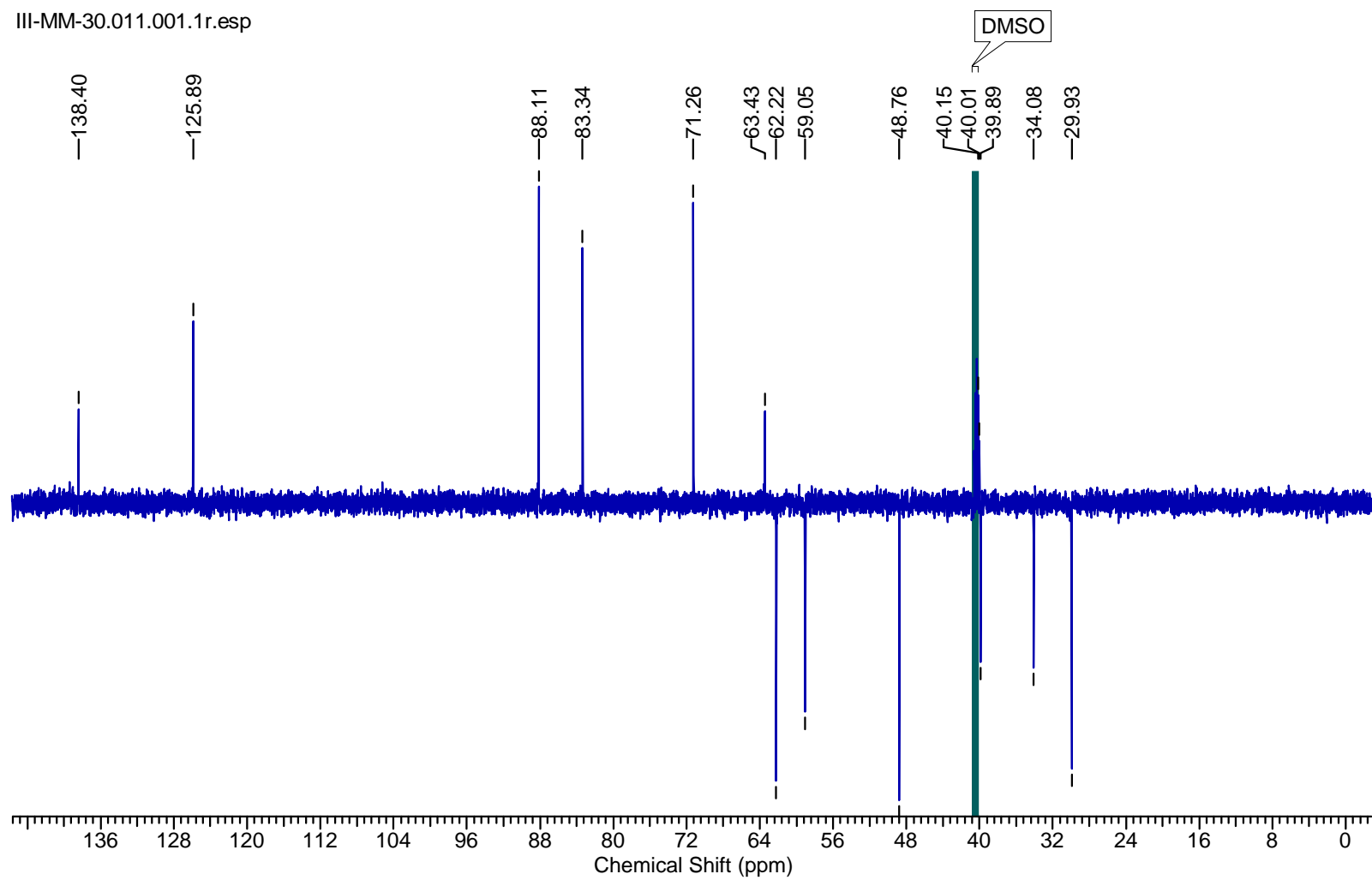


Figure S82. DEPT-135 spectrum of compound **26**.

III-MM-30-BOR.004.001.1r.esp

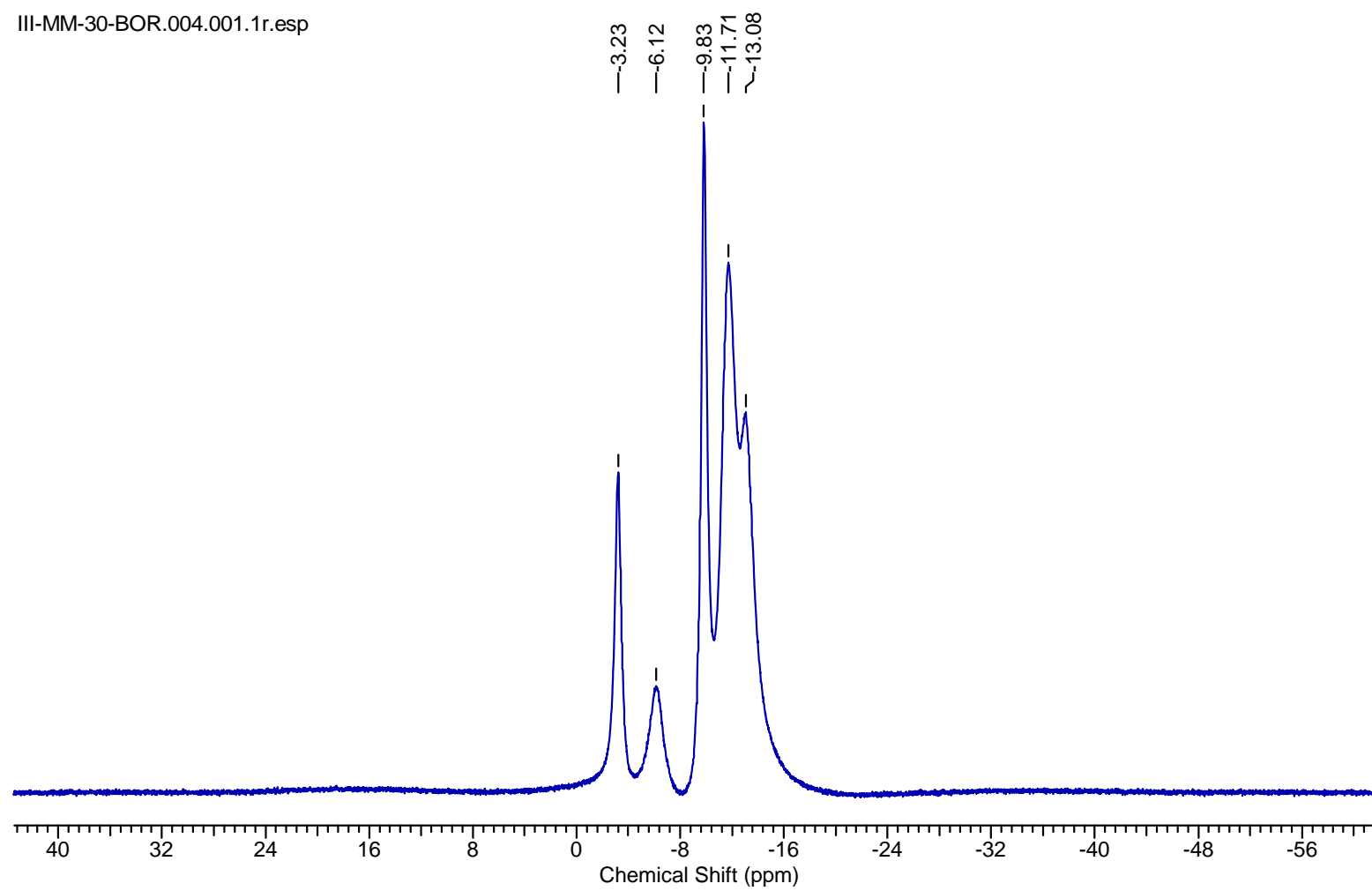


Figure S83. $^{11}\text{B}\{^1\text{H BB}\}$ NMR spectrum of compound **26**.

III-MM-30-BOR.005.001.1r.esp

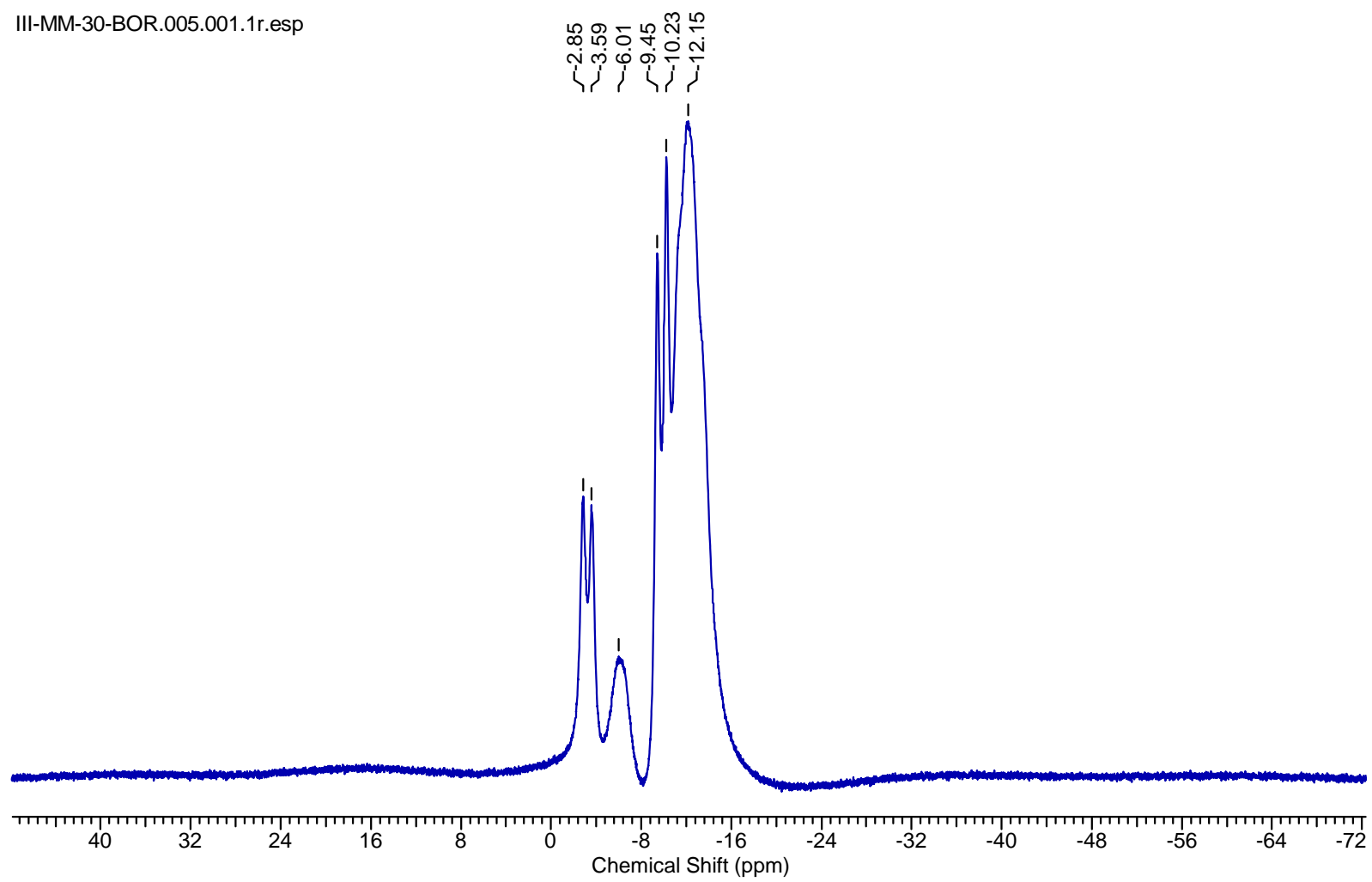


Figure S84. ^{11}B NMR spectrum of compound **26**.

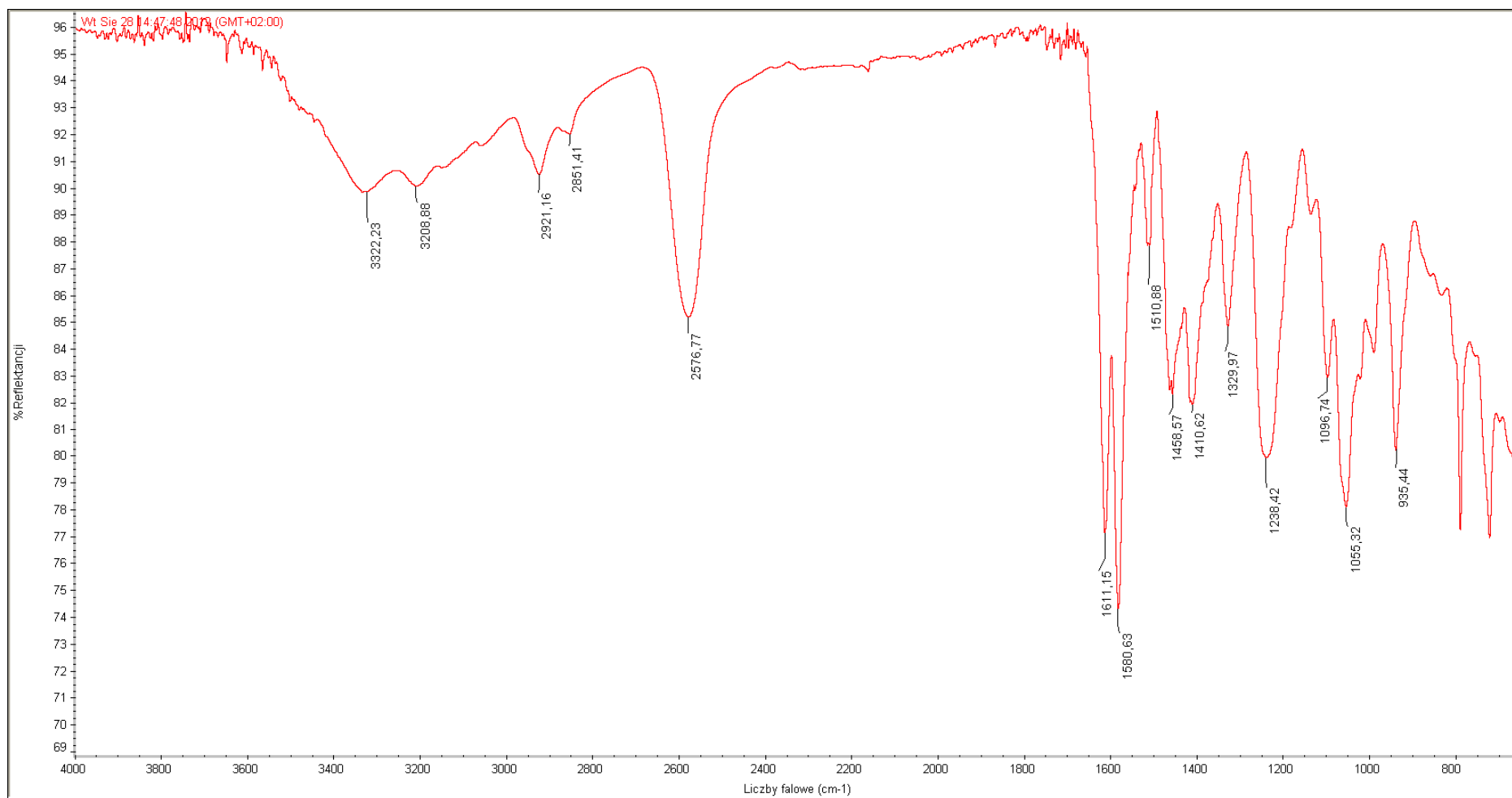
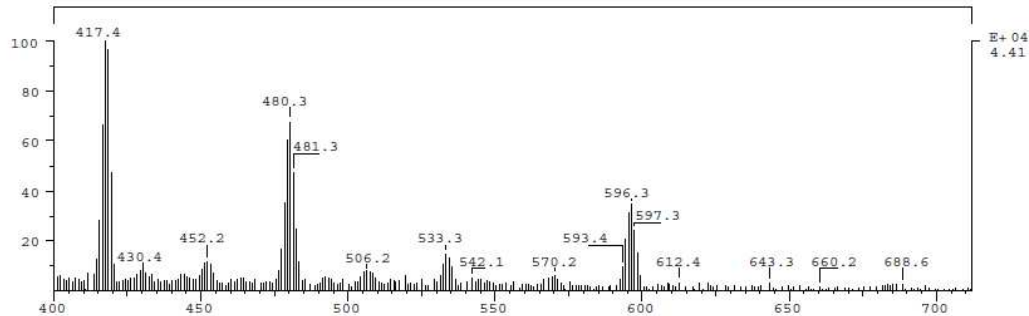
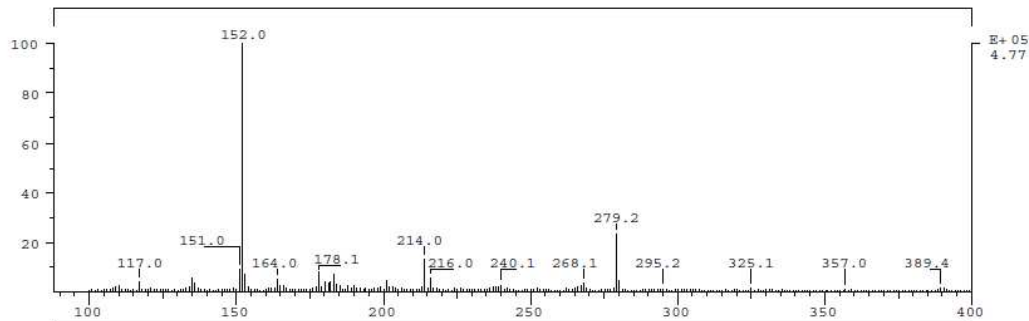


Figure S85. IR spectrum of compound **26**.

SPEC: ax501ibm 24-May-12 REG : 00:16.4 #9
 Samp: III-MM-10 Start : 14:39:56 10
 Comm: LSI, Cs+ 13 keV, gly
 Mode: FAB +VE +LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ed Client: IBM A.Olejniczak Inlet :
 Base: 152.0 Inten : 477149 Masses: 100 > 1000
 Norm: 152.0 RIC : 3061969 #peaks: 698
 Peak: 1000.00 mmu
 Data: +1>10



SPEC: ax501ibm_a 24-May-12 REG : 00:16.4 #9
 Samp: III-MM-10 Start : 14:45:25 10
 Comm: LSI, Cs+ 13 keV, gly
 Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ed Client: IBM A.Olejniczak Inlet :
 Base: 183.0 Inten : 52825 Masses: 100 > 1000
 Norm: 183.0 RIC : 466151 #peaks: 372
 Peak: 1000.00 mmu
 Data: +1>10

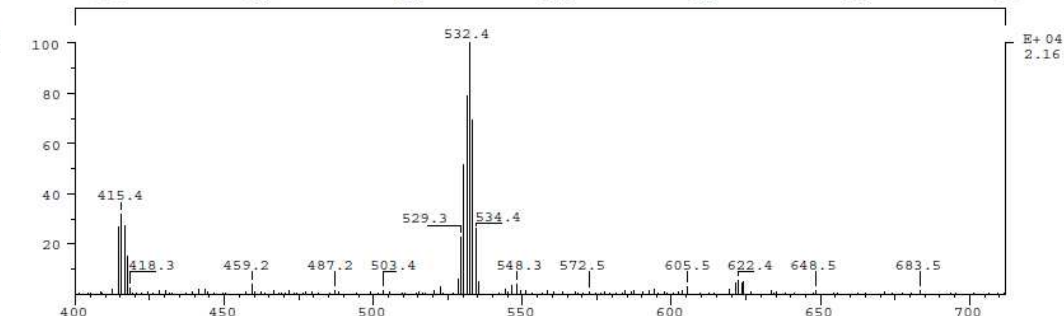
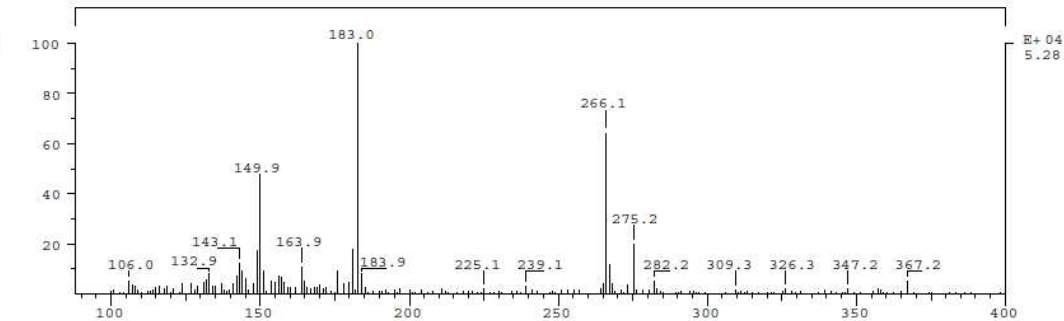


Figure S86. MS-FAB spectra of compound **26**.

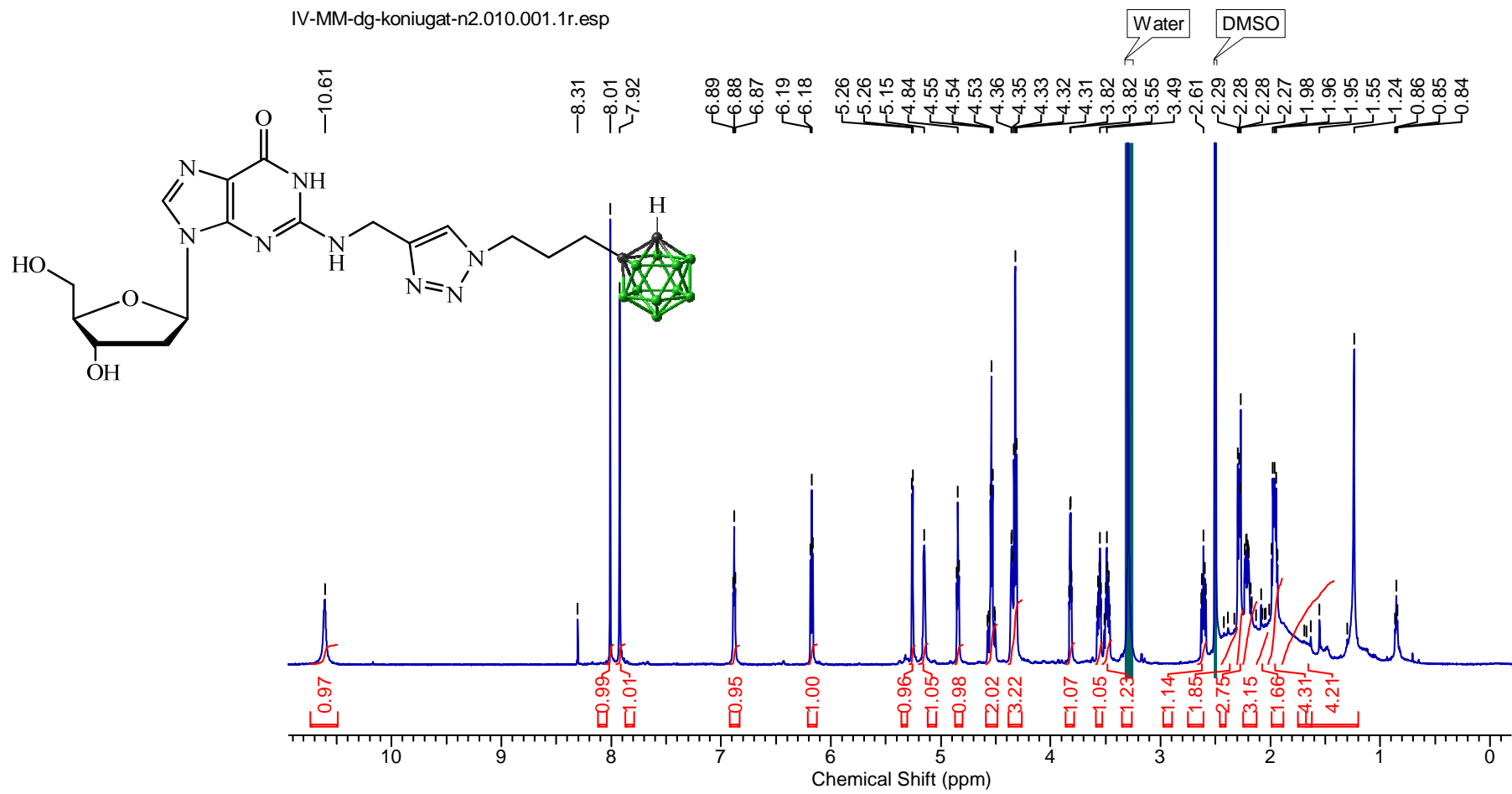


Figure S87. ^1H NMR spectrum of compound 27.

IV-MM-dg-koniugat-n2.012.001.1r.esp

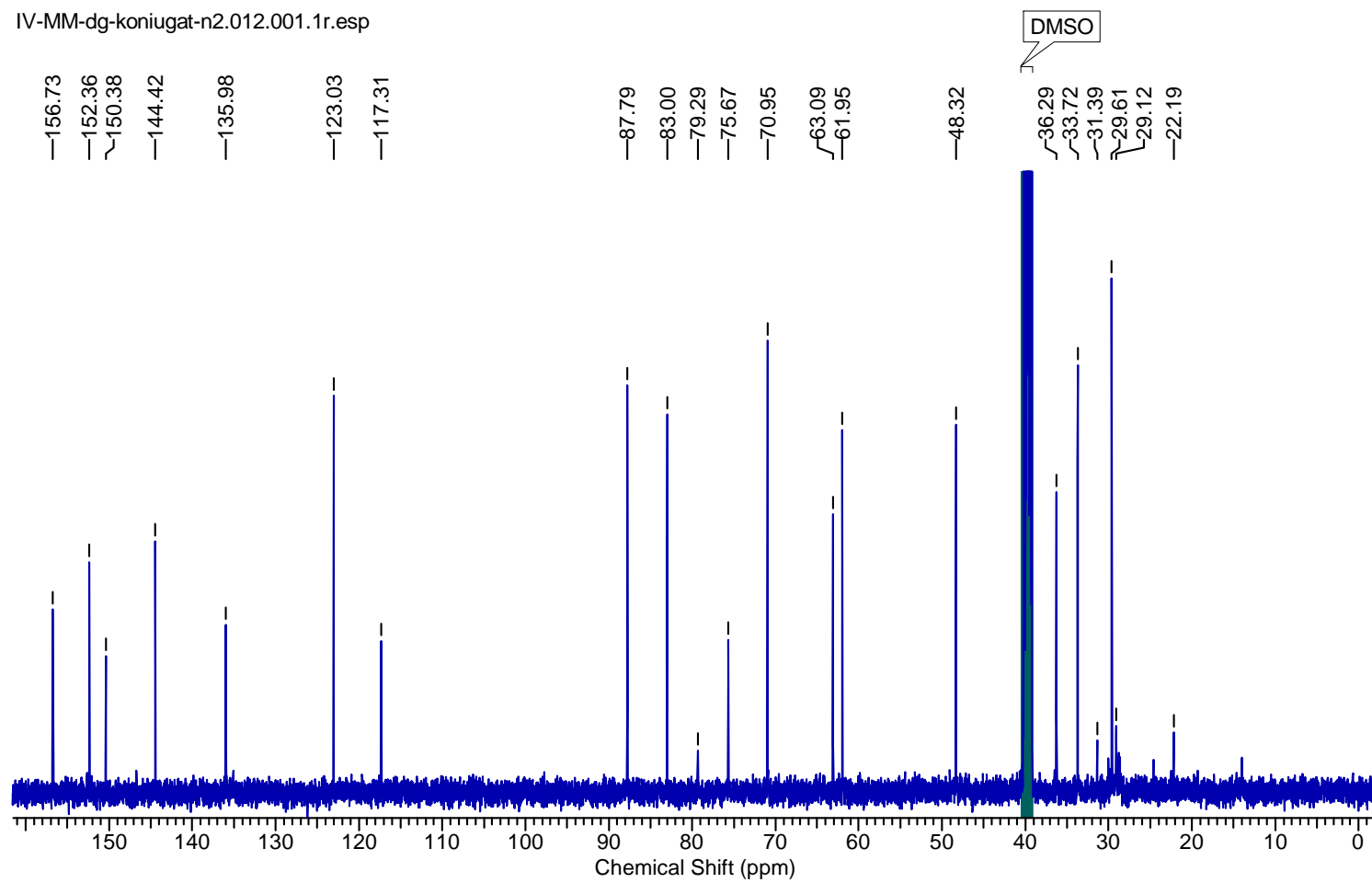


Figure S88. ^{13}C NMR spectrum of compound **27**.

IV-MM-dg-koniugat-n2.013.001.1r.esp

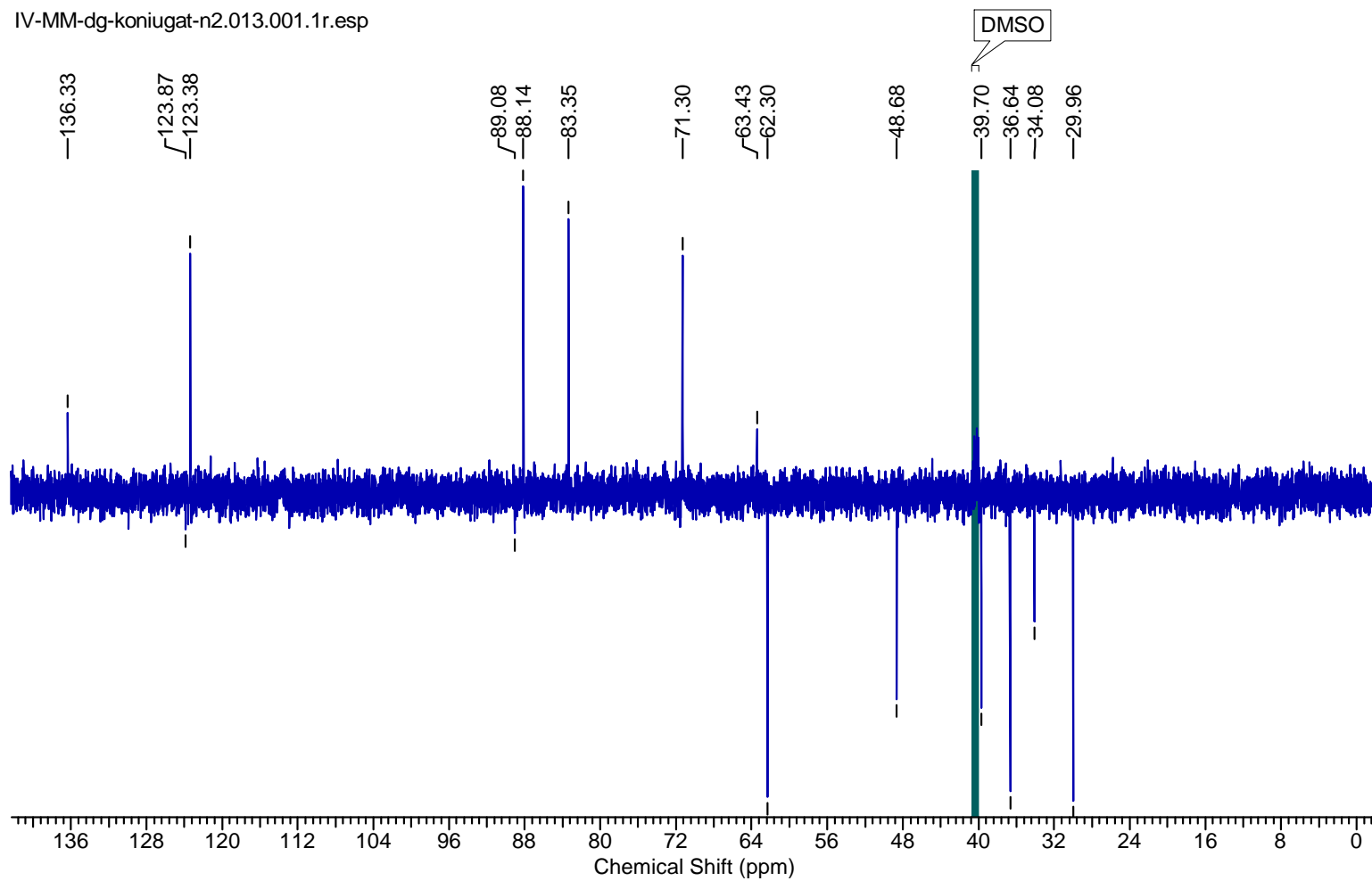


Figure S89. DEPT-135 spectrum of compound **27**.

IV-MM-amido-dg-koniugat-n2.007.001.1r.esp

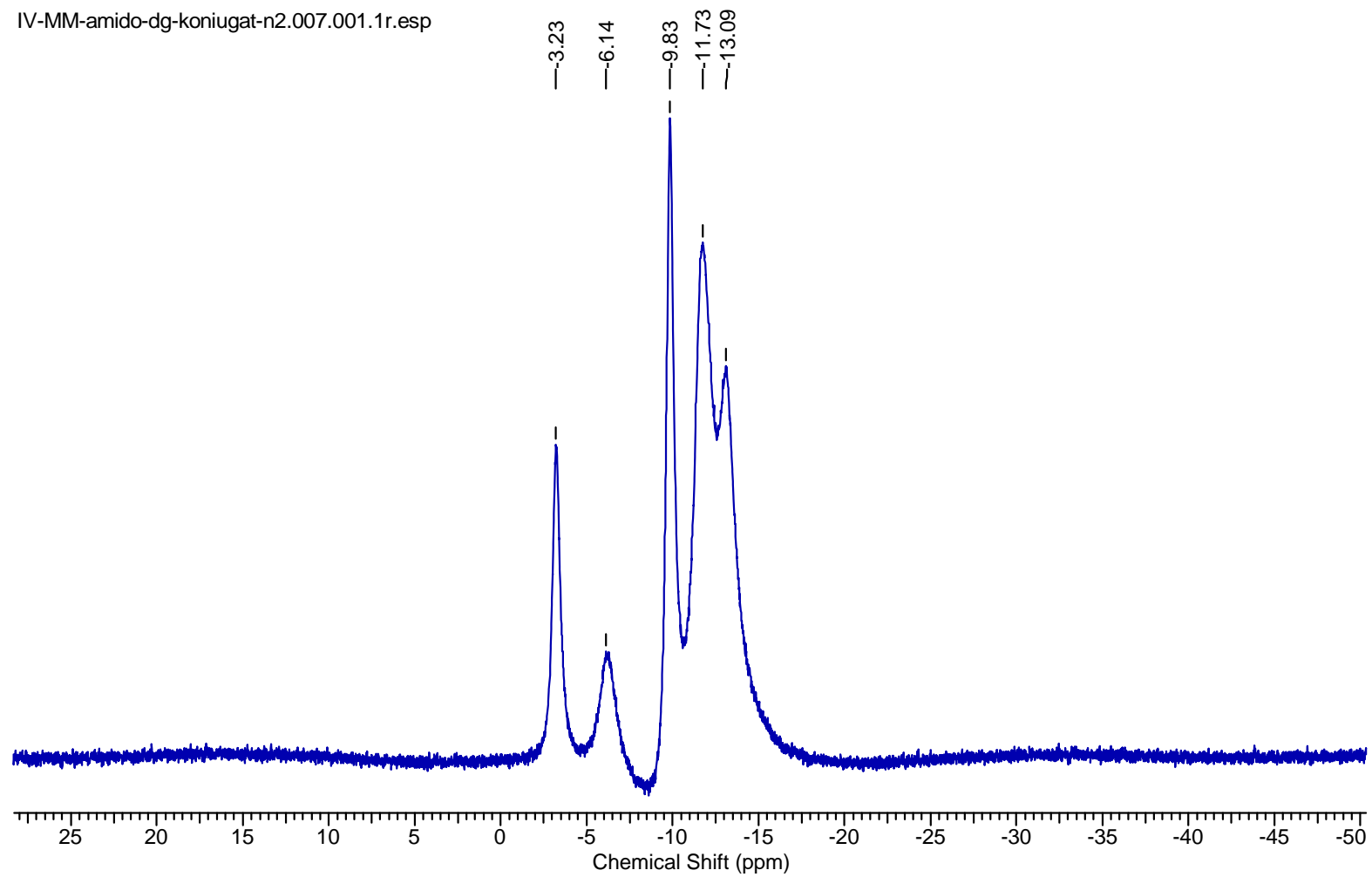


Figure S90. $^{11}\text{B}\{^1\text{H BB}\}$ NMR spectrum of compound **27**.

IV-MM-amido-dg-koniugat-n2.008.001.1r.esp

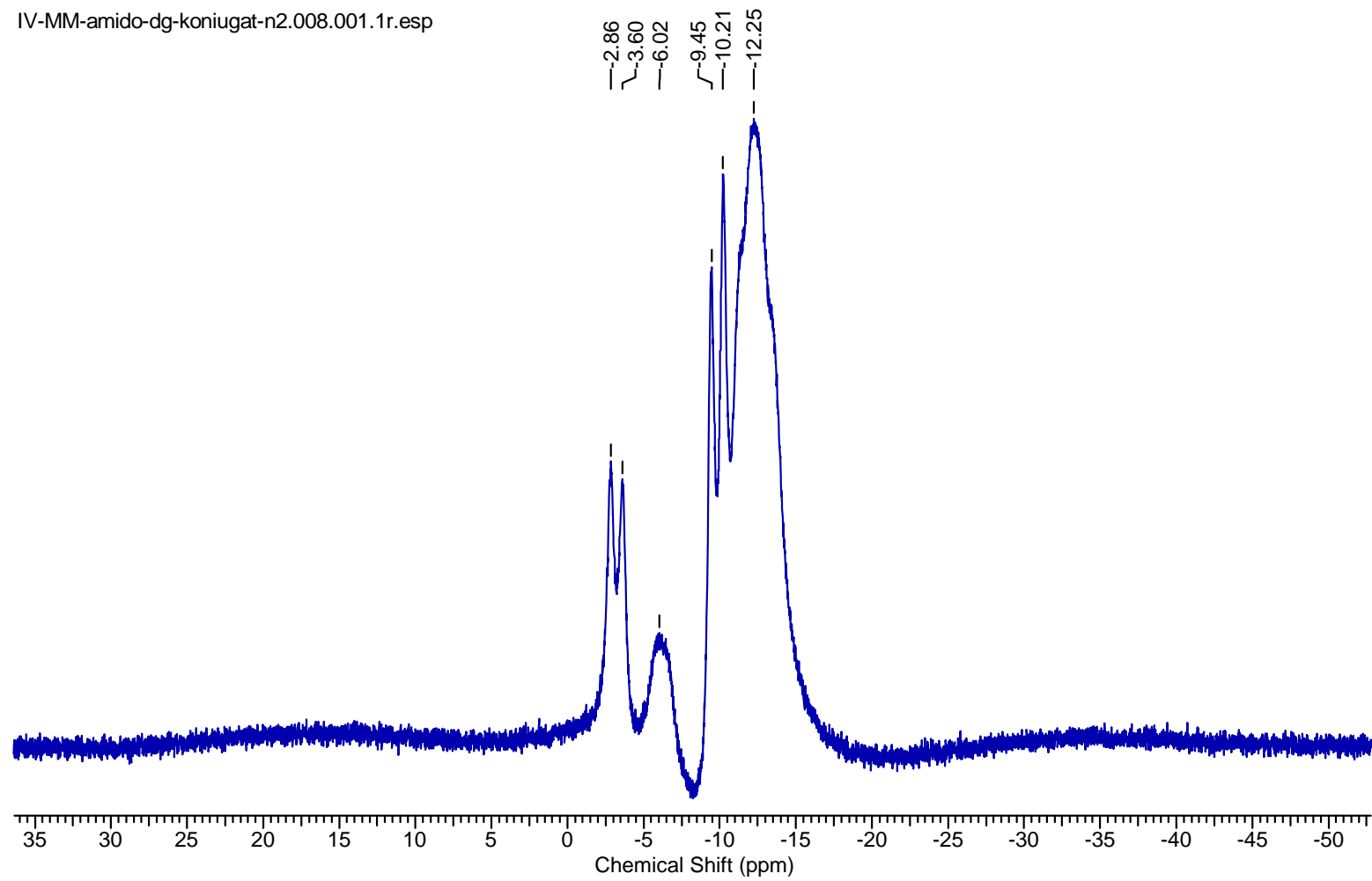


Figure S91. ^{11}B NMR spectrum of compound **27**.

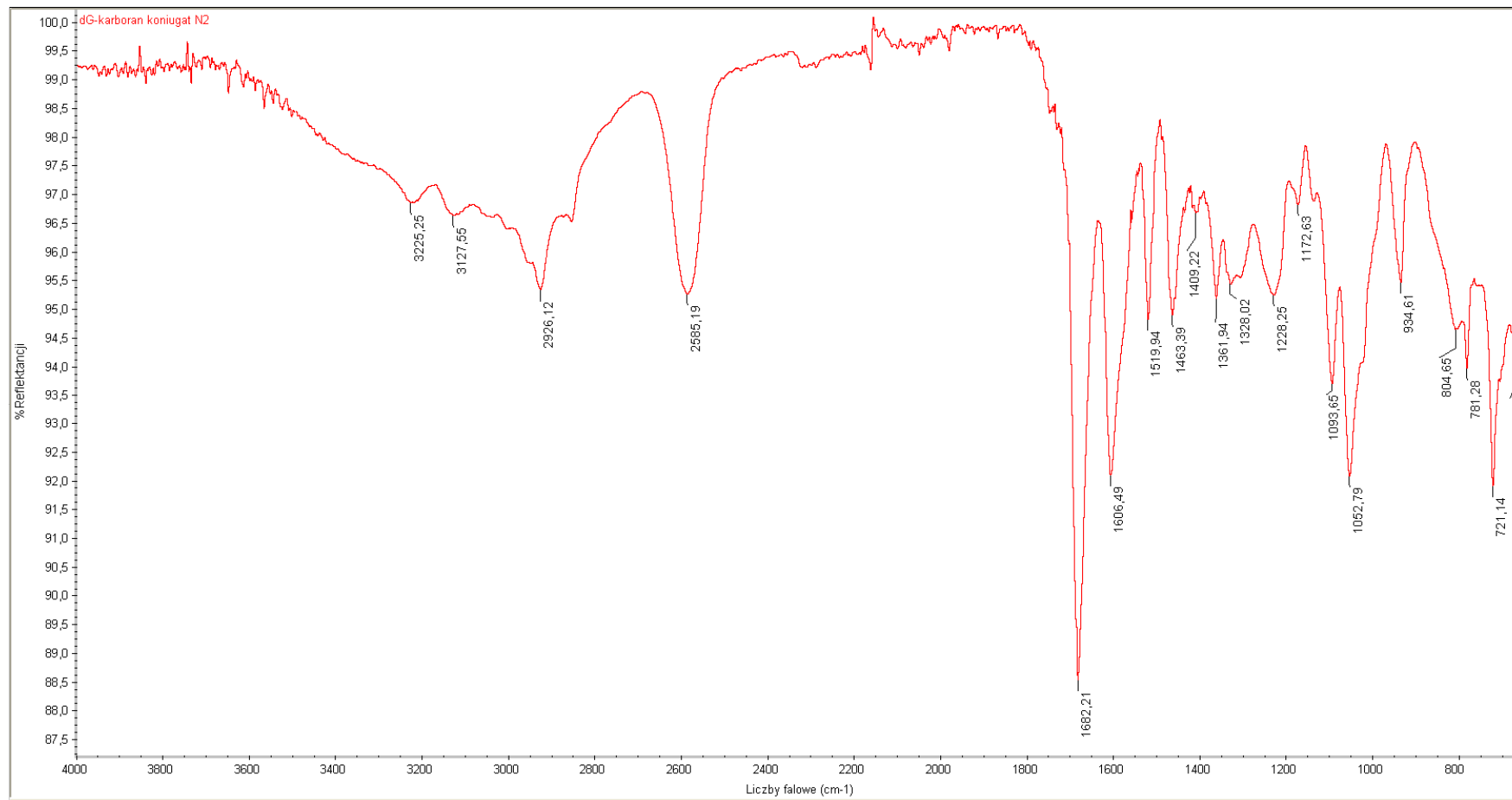


Figure S92. IR spectrum of compound 27.

SPEC: az437ibm 17-Dec-13 REG : 00:16.4 #9
 Samp: dG-karboran-N2 Start : 13:52:10 10
 Comm: LSI, Cs+ 13 keV, gly
 Mode: FAB +VE +LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ub Client: IBM A.Olejniczak Inlet :
 Base: 185.1 Inten : 260484 Masses: 100 > 1000
 Norm: 185.1 RIC : 2689202 #peaks: 608
 Peak: 1000.00 mmu
 Data: +1>10

SPEC: az437ibm_b 17-Dec-13 REG : 00:16.4 #9
 Samp: dG-karboran-N2 Start : 15:37:53 10
 Comm: LSI, Cs+ 13 keV, gly
 Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ub Client: IBM A.Olejniczak Inlet :
 Base: 183.0 Inten : 106048 Masses: 100 > 1000
 Norm: 183.0 RIC : 2216830 #peaks: 778
 Peak: 1000.00 mmu
 Data: +1>10

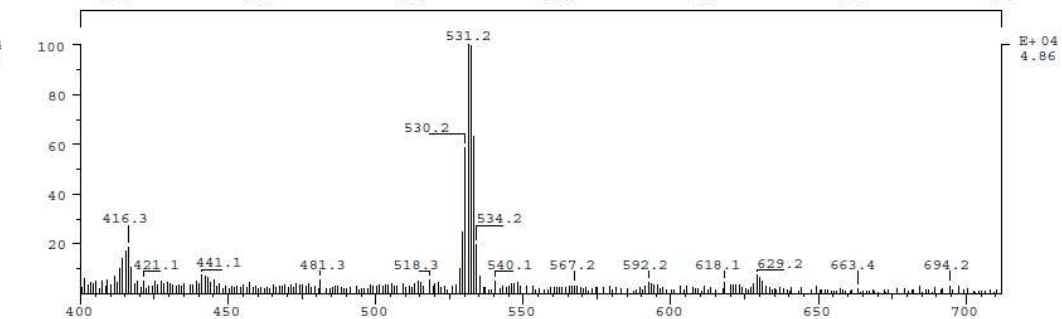
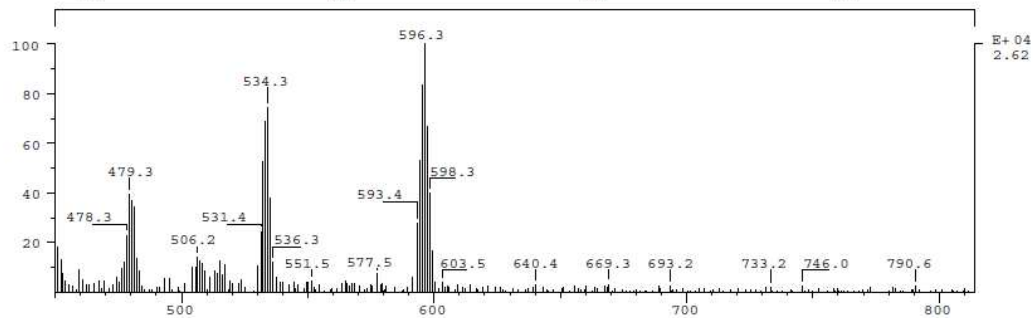
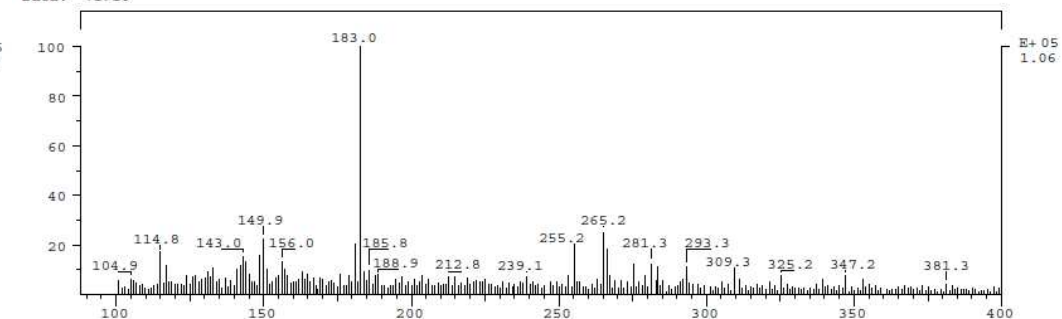
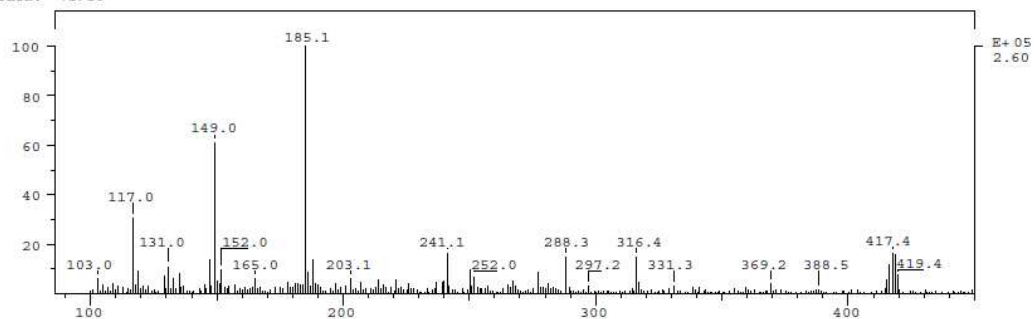


Figure S93. MS-FAB spectra of compound 27.

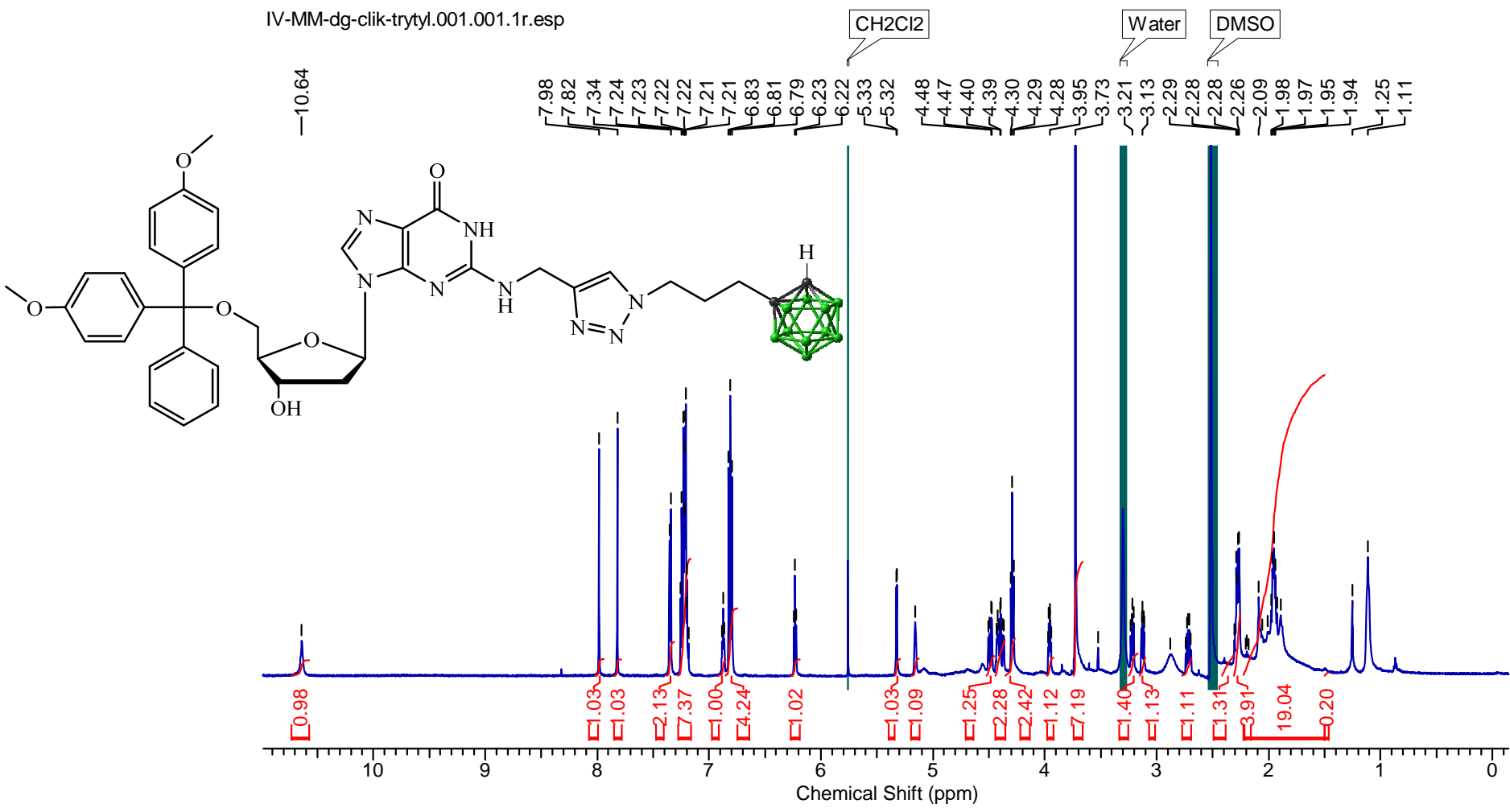


Figure S94. ¹H NMR spectrum of compound 28.

IV-MM-dg-clik-trytyl.012.001.1r.esp

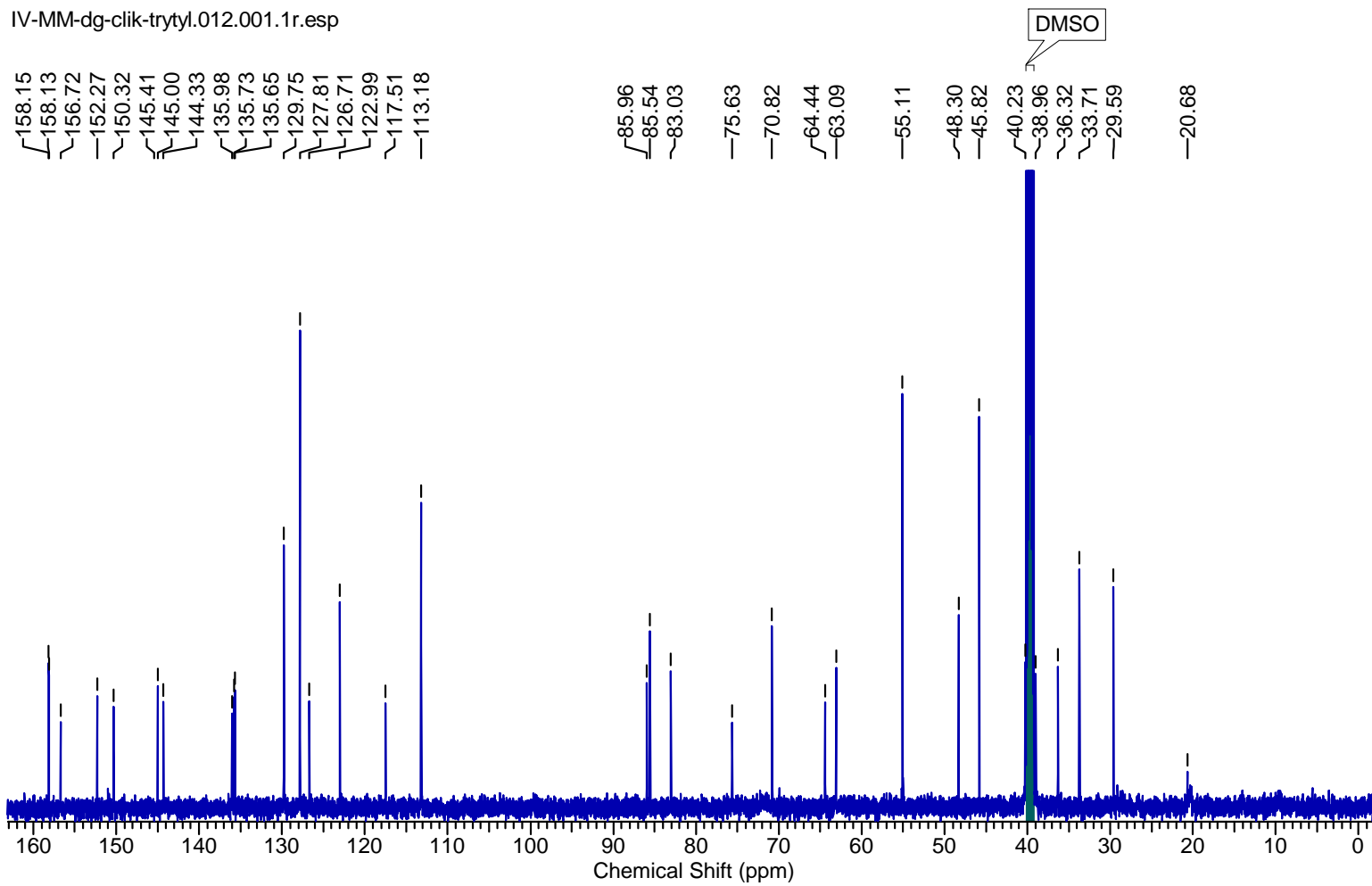


Figure S95. ^{13}C NMR spectrum of compound 28.

IV-MM-dg-clik-trytyl.013.001.1r.esp

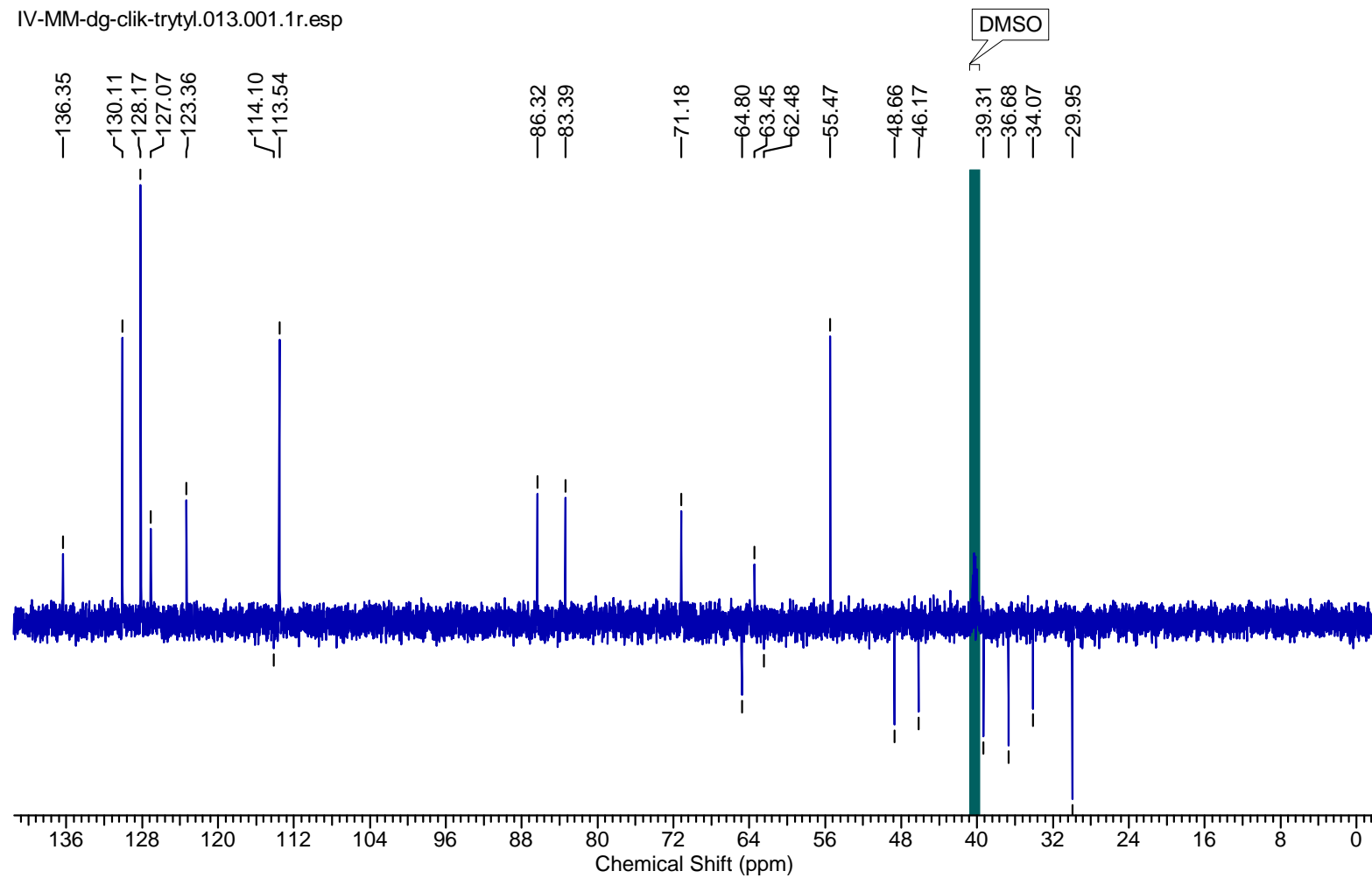


Figure S96. DEPT-135 spectrum of compound **28**.

IV-MM-amido-dg-clik-trytyl.007.001.1r.esp

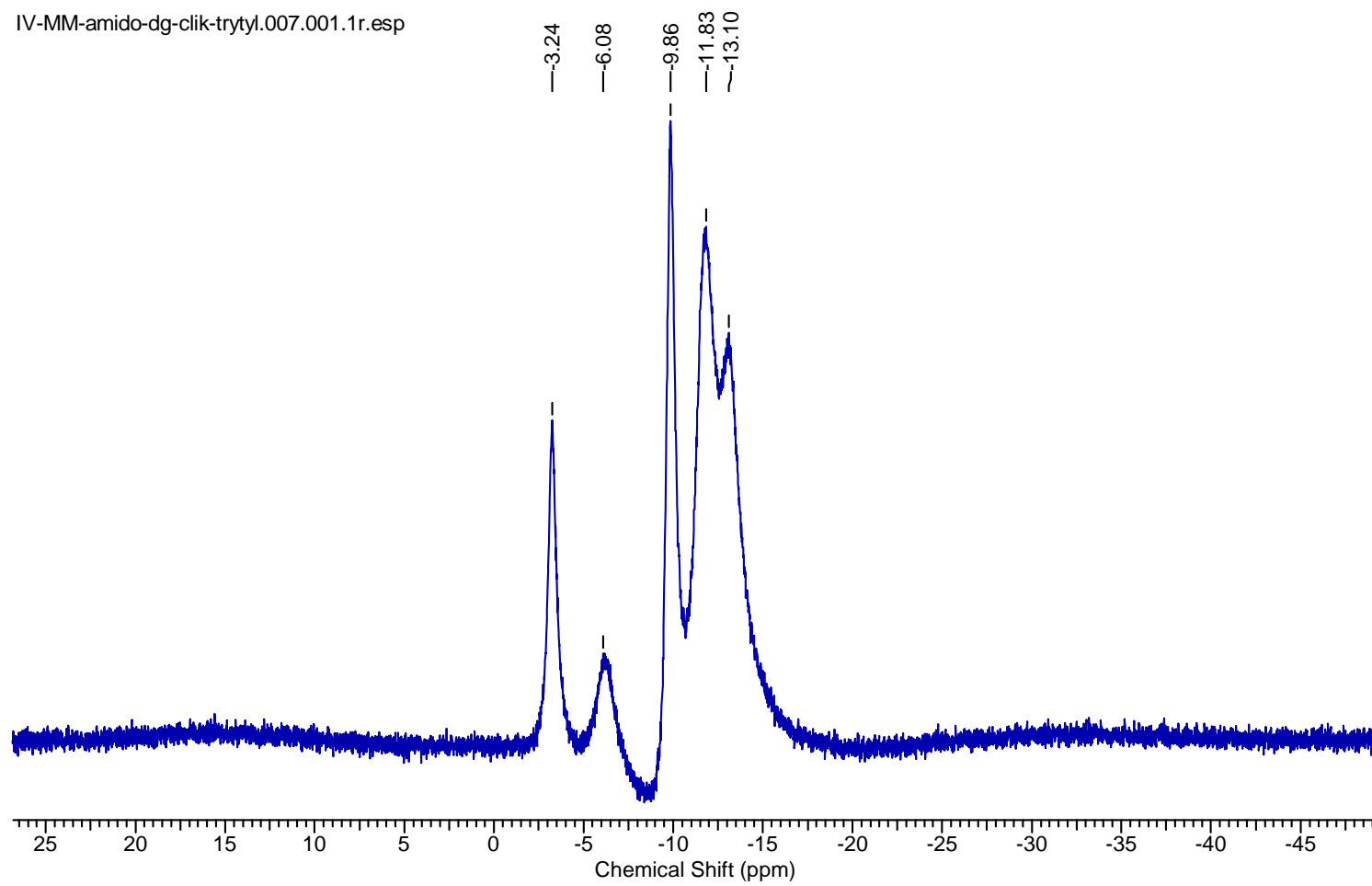


Figure S97. $^{11}\text{B}\{^1\text{H BB}\}$ NMR spectrum of compound **28**.

IV-MM-amido-dg-clik-trytyl.008.001.1r.esp

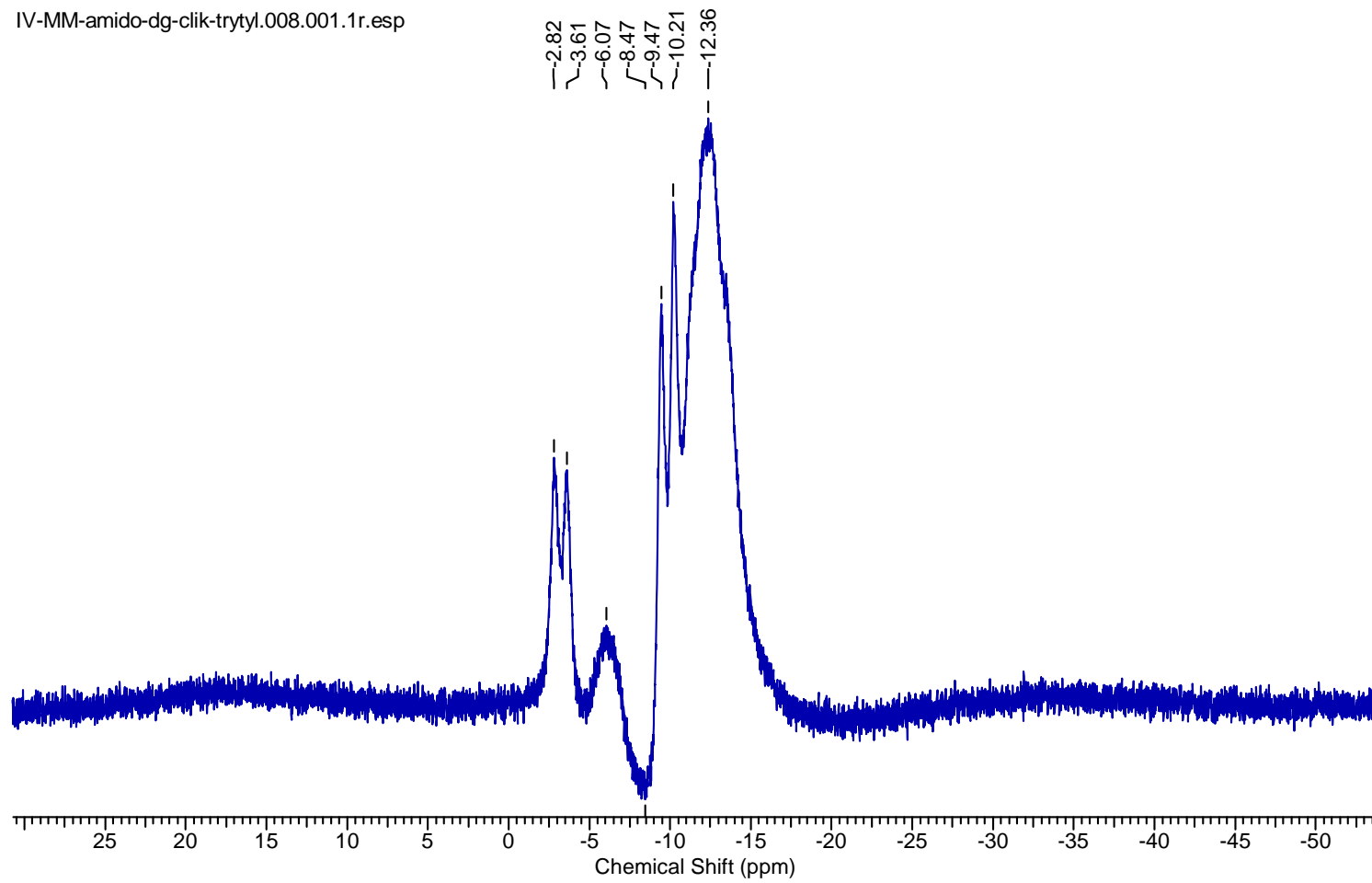


Figure S98. ^{11}B NMR spectrum of compound **28**.

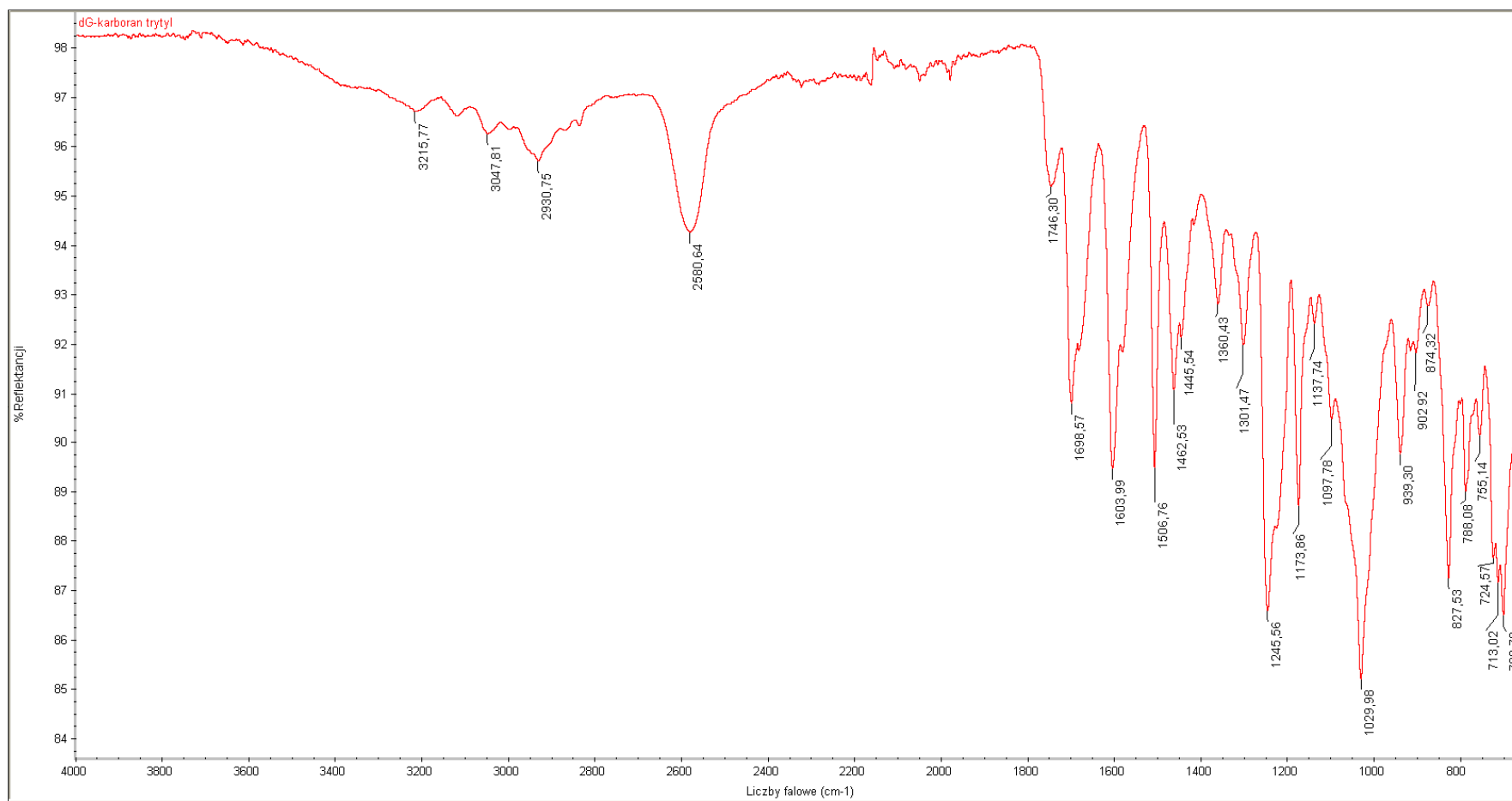


Figure S99. IR spectrum of compound **28**.

SPEC: az438ibm 17-Dec-13 REG : 00:16.4 #9
 Samp: dG-karboran-N2-trytyl Start : 14:50:31 10
 Comm: LSI, Cs+ 13 keV, gly
 Mode: FAB +VE +LMR BSCAN (EXP) UP LR NRM Study : MS CBM1M PAN Lodz
 Oper: ub Client: IBM A.Olejniczak Inlet :
 Base: 303.2 Inten : 25521140 Masses: 100 > 1000
 Norm: 303.2 RIC : 52998745 #peaks: 793
 Peak: 1000.00 mmu
 Data: +1>10

SPEC: az438ibm_c 17-Dec-13 REG : 00:16.4 #9
 Samp: dG-karboran-N2-trytyl Start : 16:20:29 10
 Comm: LSI, Cs+ 13 keV, gly
 Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBM1M PAN Lodz
 Oper: ub Client: IBM A.Olejniczak Inlet :
 Base: 182.9 Inten : 2006159 Masses: 100 > 1000
 Norm: 182.9 RIC : 12754517 #peaks: 854
 Peak: 1000.00 mmu
 Data: +1>10

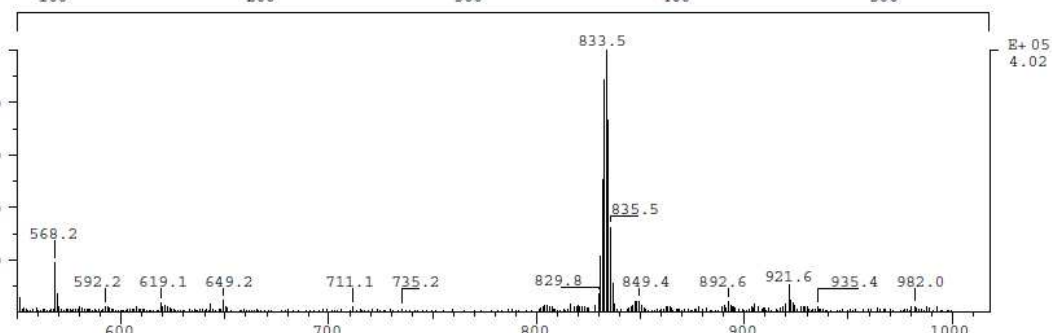
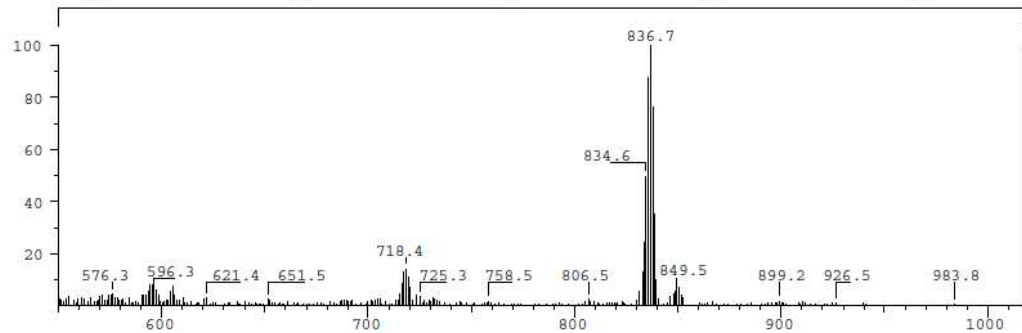
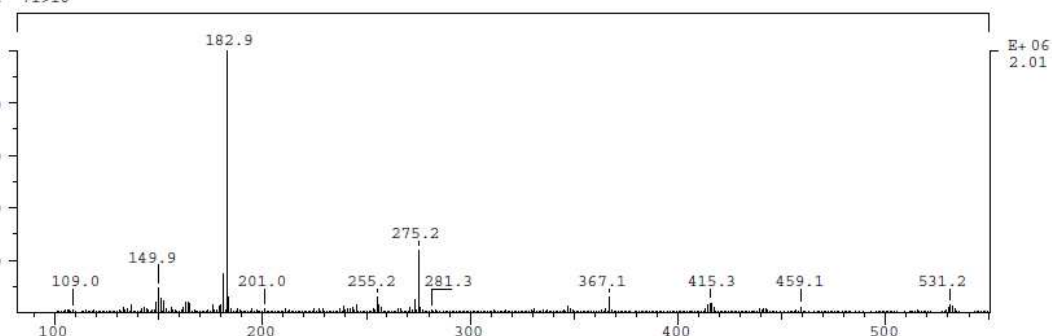
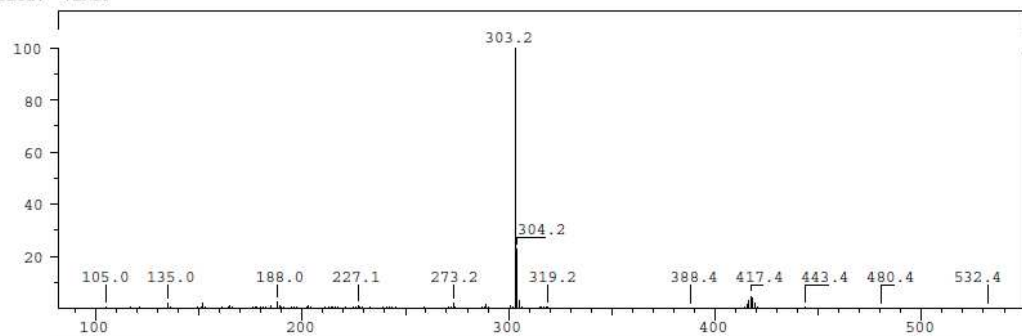


Figure S100. MS-FAB spectra of compound 28.

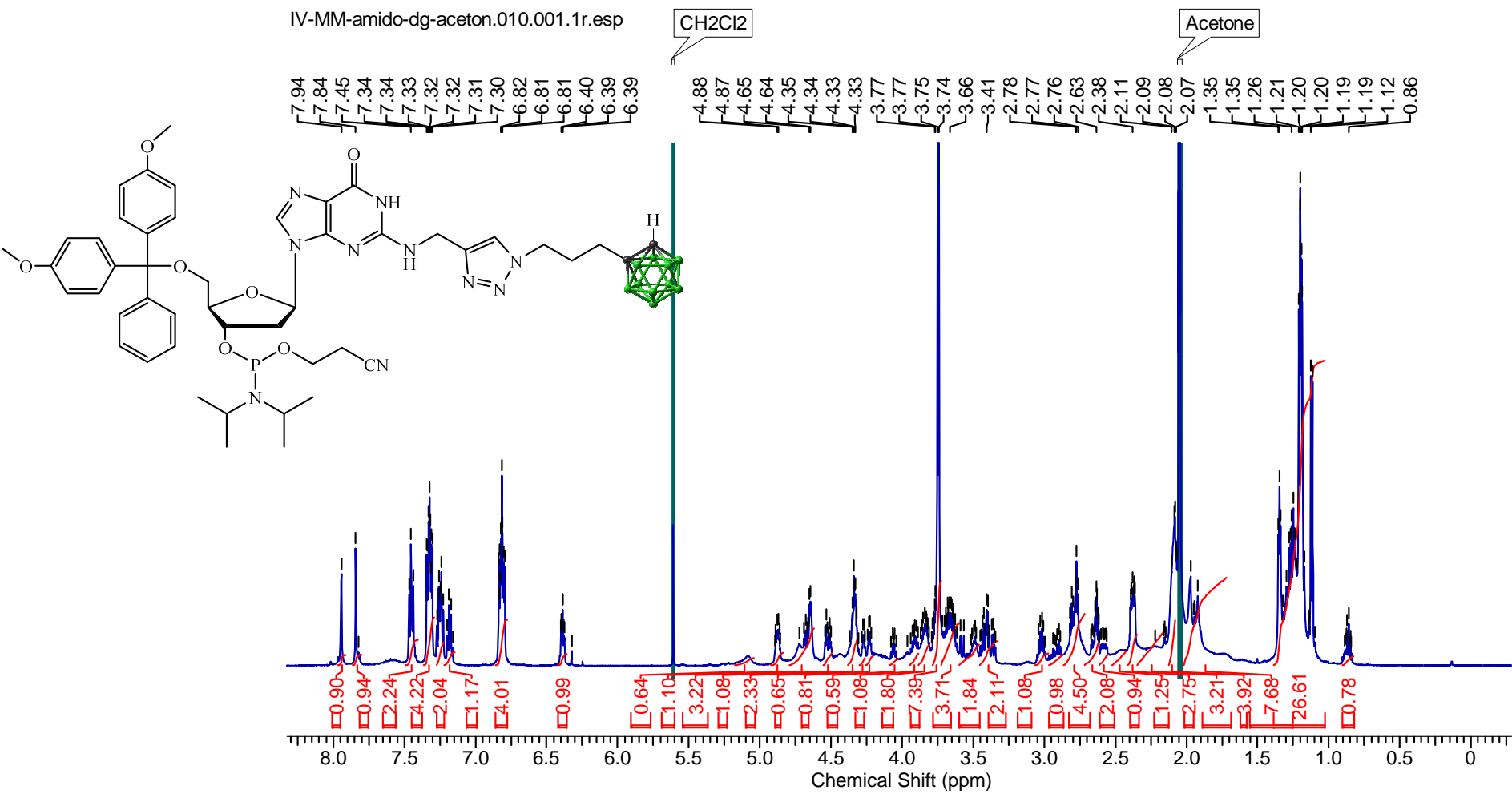


Figure S101. ¹H NMR spectrum of compound 32.

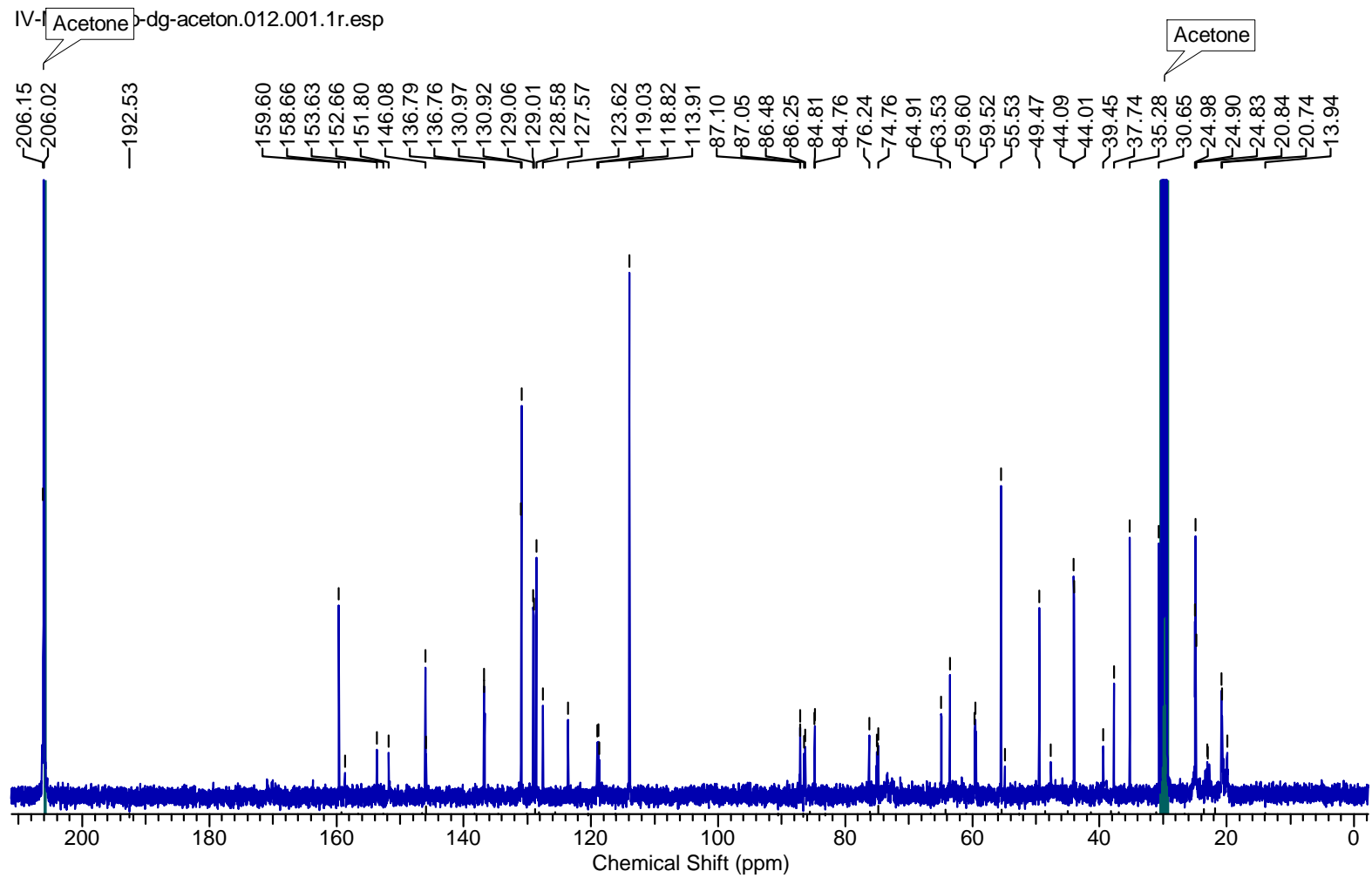


Figure S102. ^{13}C NMR spectrum of compound 32.

IV-MM-amido-dg-aceton.013.001.1r.esp

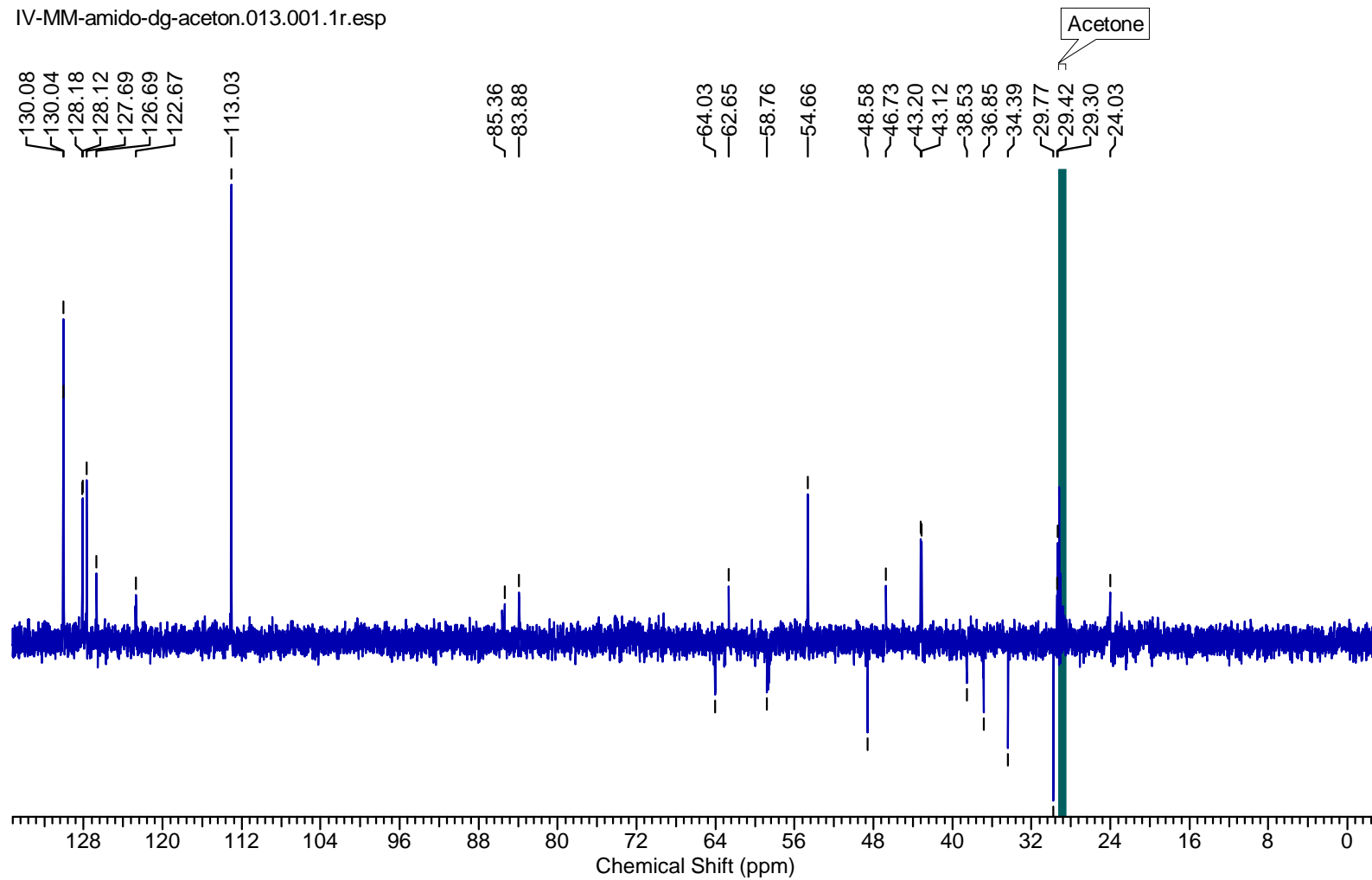


Figure S103. DEPT-135 spectrum of compound **32**.

IV-MM-amido-dg-aceton.007.001.1r.esp

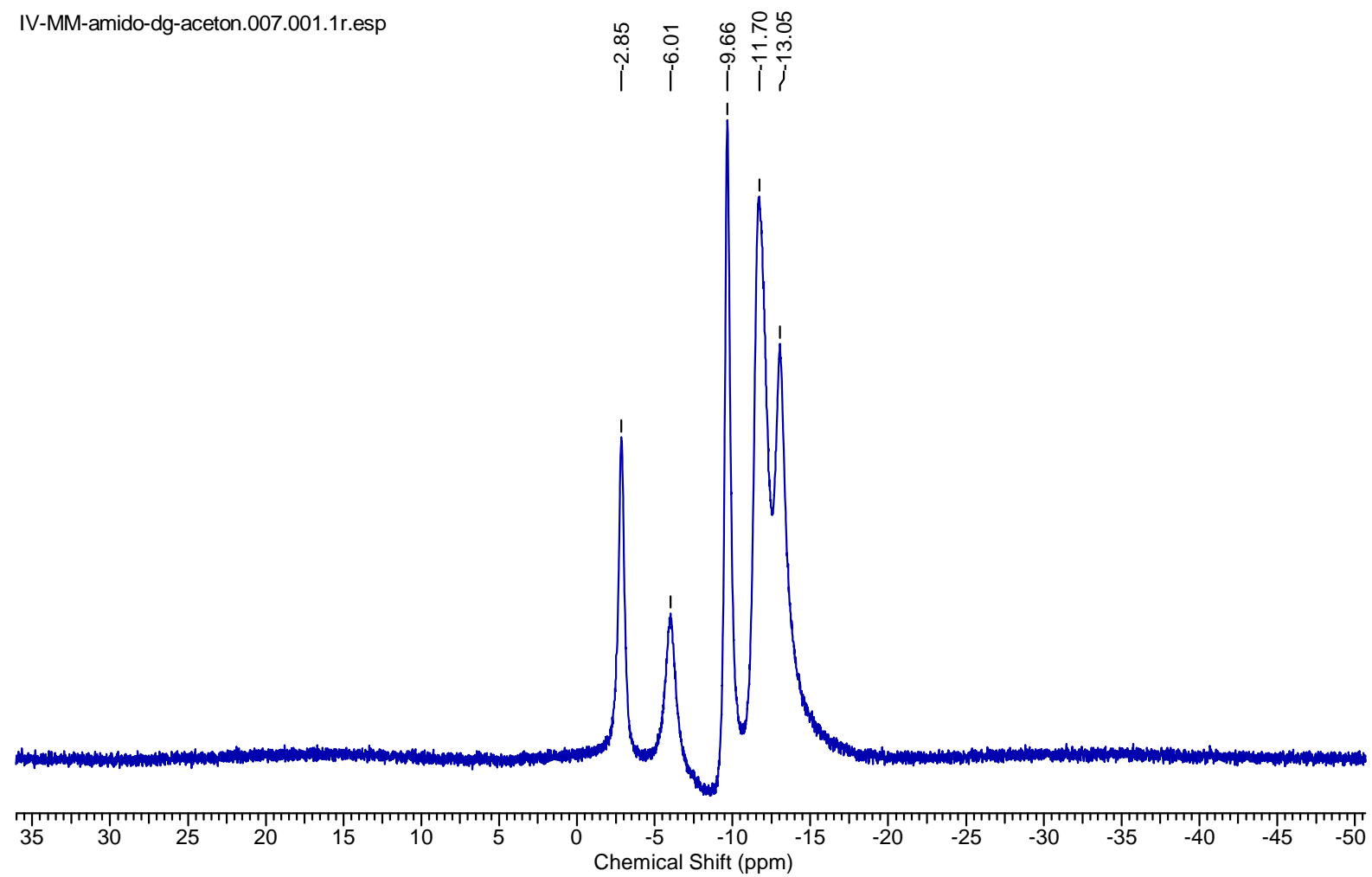


Figure S104. $^{11}\text{B}\{^1\text{H BB}\}$ NMR spectrum of compound **32**.

IV-MM-amido-dg-aceton.008.001.1r.esp

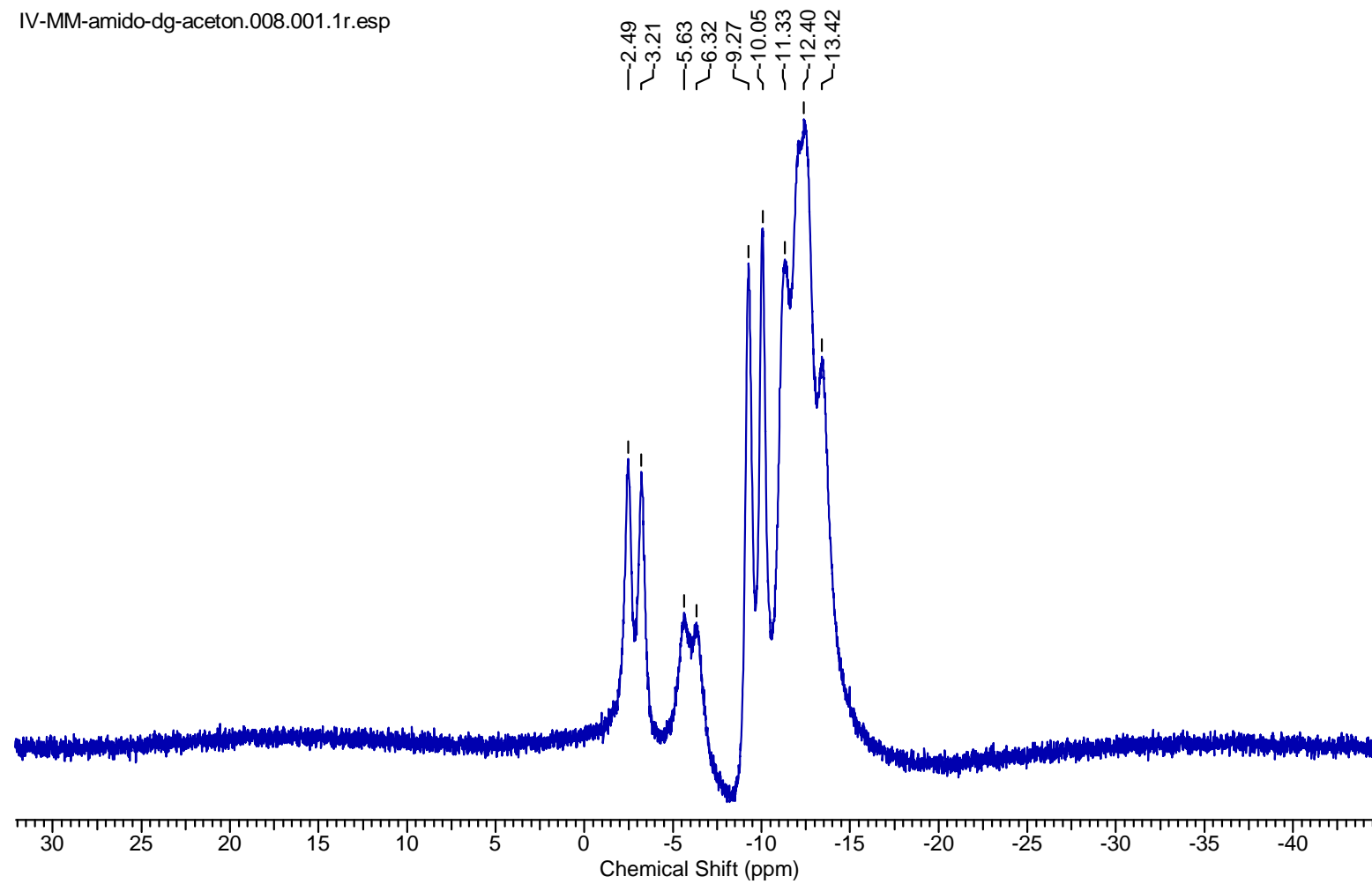


Figure S105. ^{11}B NMR spectrum of compound **32**.

II-MM-amido-dg-aceton.001.001.1r.esp

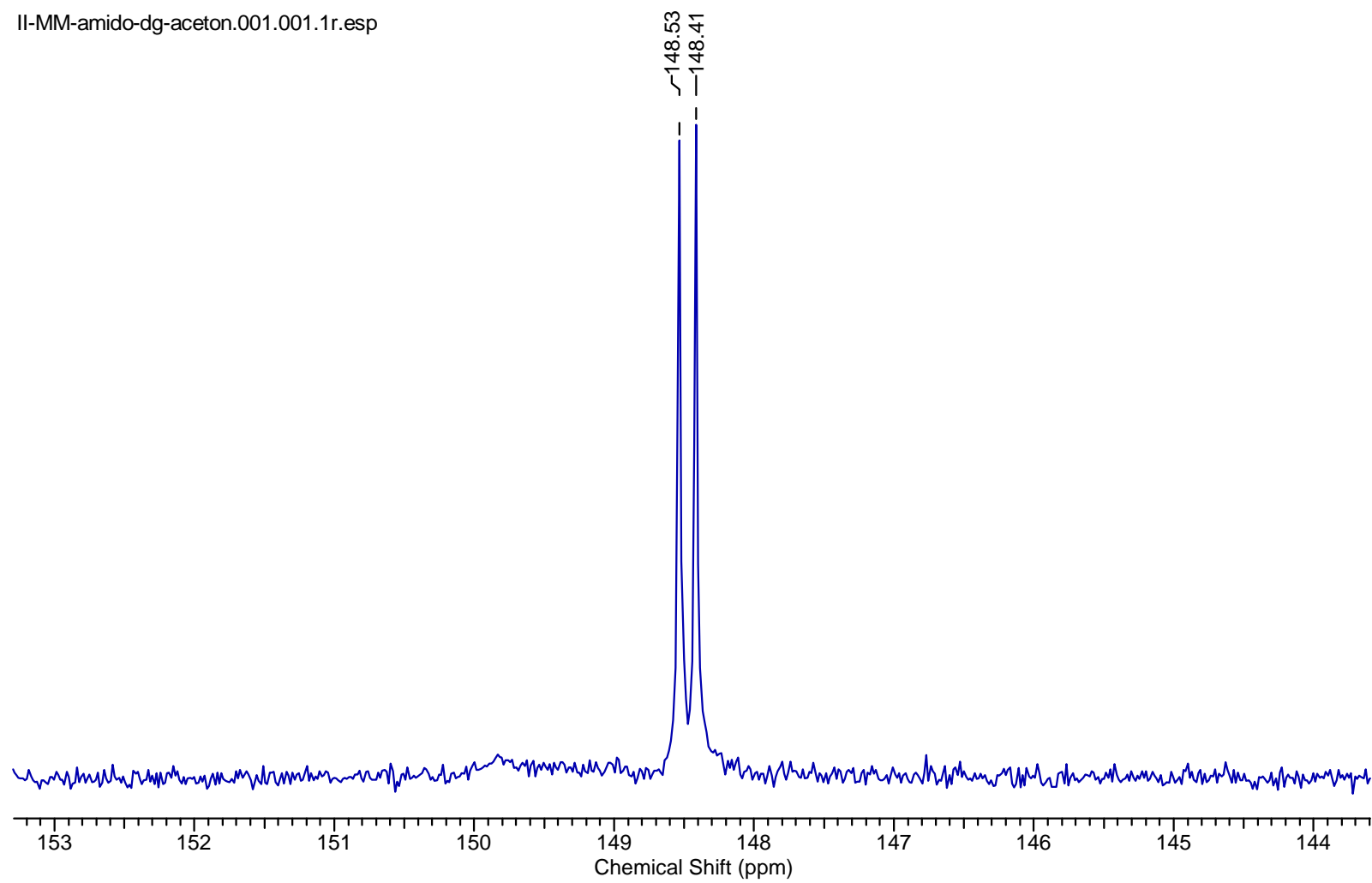


Figure S106. ^{31}P NMR spectrum of compound **32**.

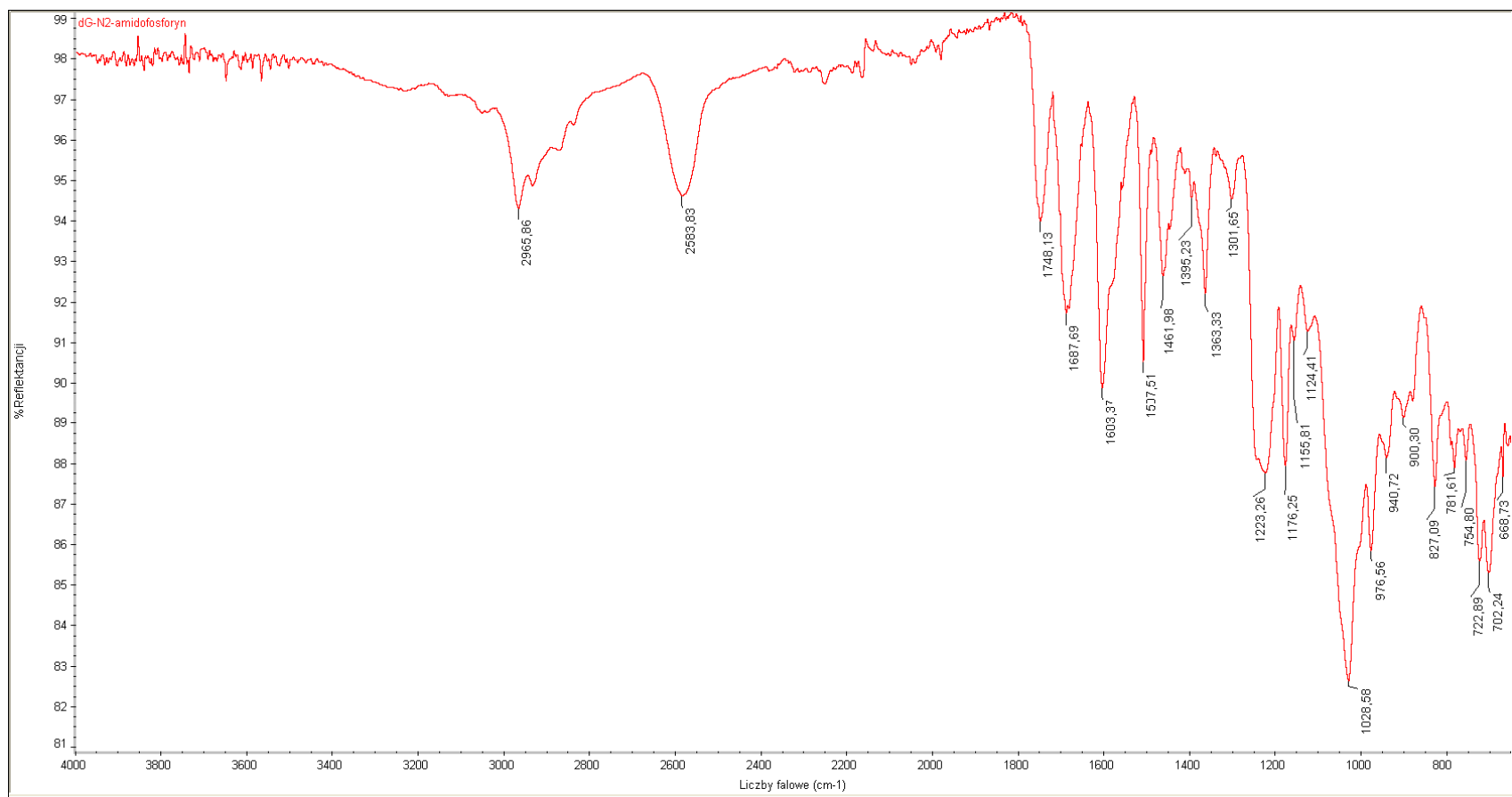
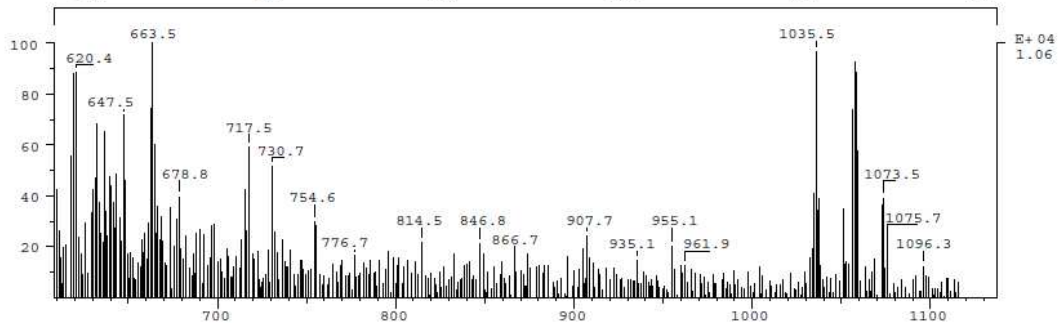
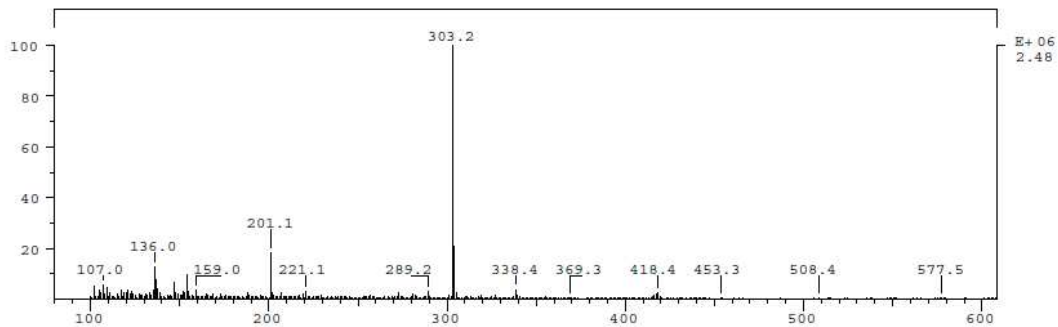


Figure S107. IR spectrum of compound 32.

SPEC: az4671bm_c 23-Dec-13 REG : 00:16.9 #9
 Samp: dg-amido LSI, Cs+ 13 keV, nba Start : 10:59:43 10
 Comm: LSI, Cs+ 13 keV, nba
 Mode: FAB +VE +LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ew Client: IBM A.Olejniczak Inlet :
 Base: 303.2 Inten : 2484027 Masses: 100 > 1117
 Norm: 303.2 RIC : 13835387 #peaks: 917
 Peak: 1000.00 mmu
 Data: +1>10



SPEC: az4671bm_b 23-Dec-13 REG : 00:16.9 #9
 Samp: dg-amido LSI, Cs+ 13 keV, nba Start : 10:56:11 10
 Comm: LSI, Cs+ 13 keV, nba
 Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ew Client: IBM A.Olejniczak Inlet :
 Base: 153.0 Inten : 2639984 Masses: 100 > 1127
 Norm: 153.0 RIC : 17142050 #peaks: 1014
 Peak: 1000.00 mmu
 Data: +1>10

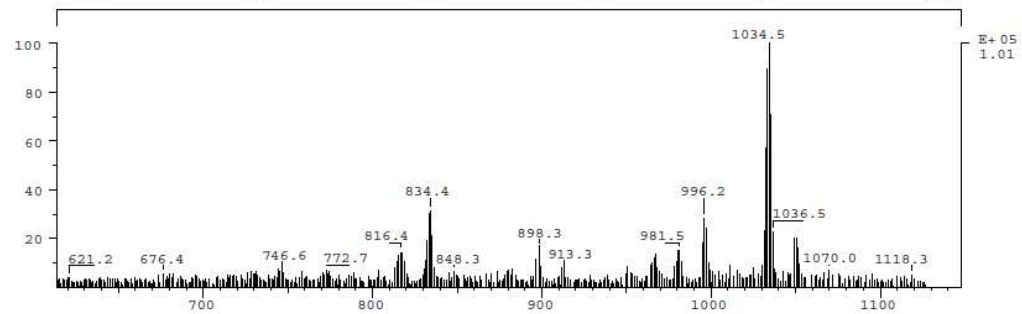
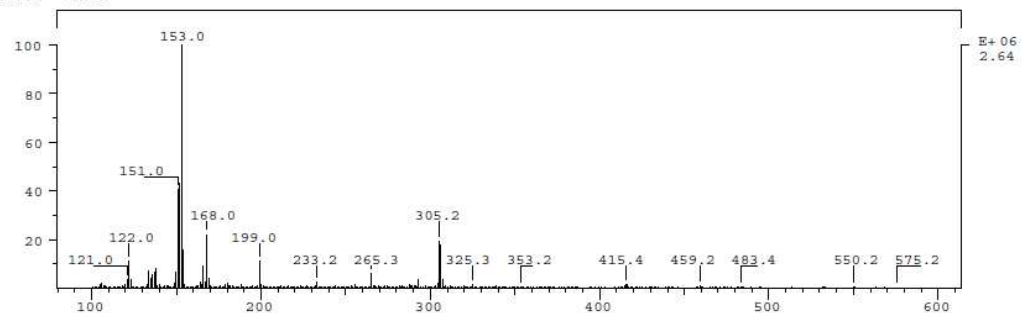


Figure S108. MS-FAB spectra of compound 32.

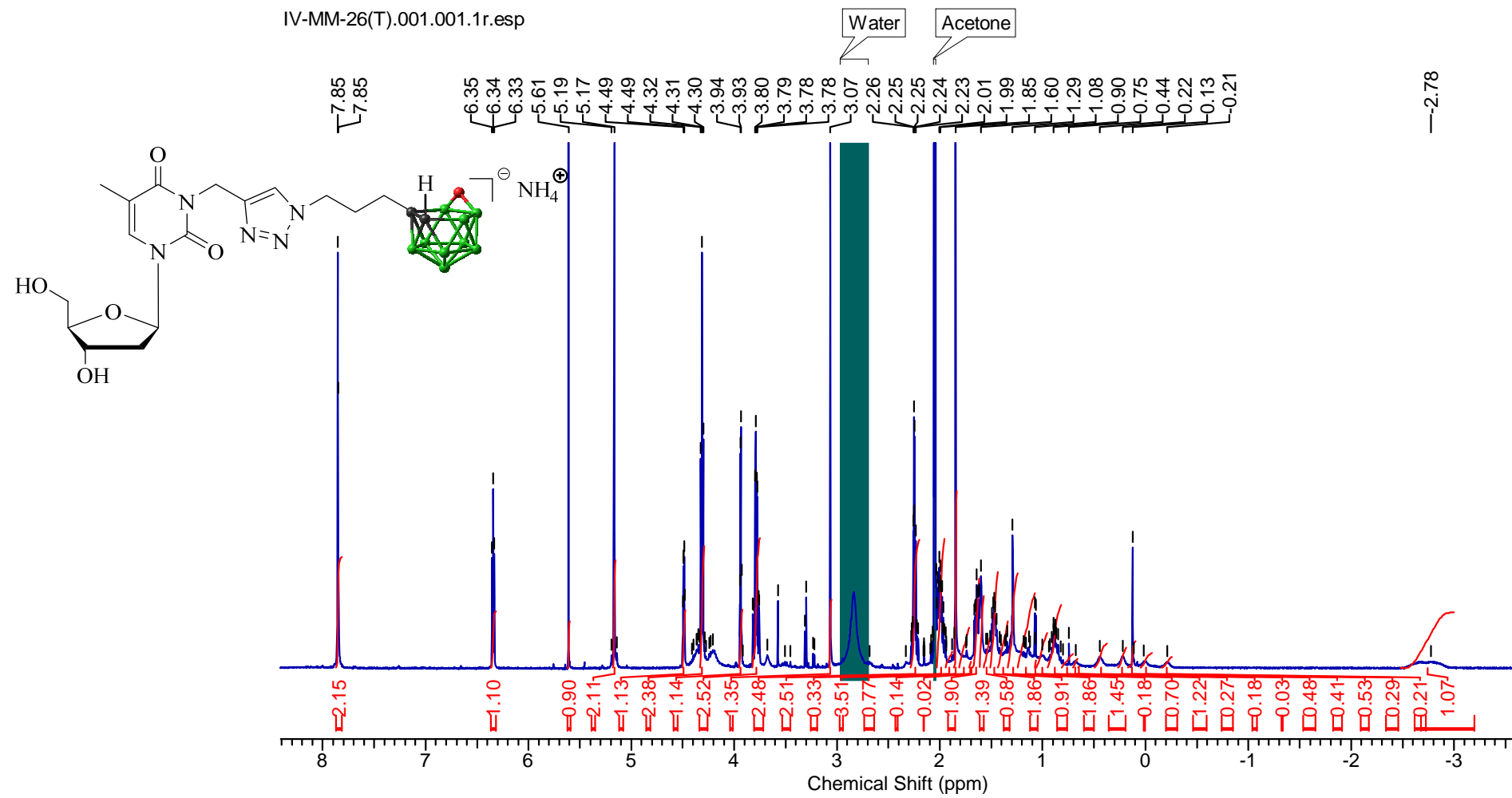


Figure S109. ^1H NMR spectrum of compound 33.

SPEC: ay3591bm_a 11-Jan-13 REG : 00:16.9 #9
Samp: T-mido Start : 15:43:52 10
Comm: LSI, Cs+ 13 keV, gly
Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
Oper: ed Client: IBM PAN A.Olejnicza Inlet :
Base: 283.4 Inten : 166018 Masses: 100 > 1117
Norm: 283.4 RIC : 3065074 #peaks: 815
Peak: 1000.00 mmu
Data: +1>10

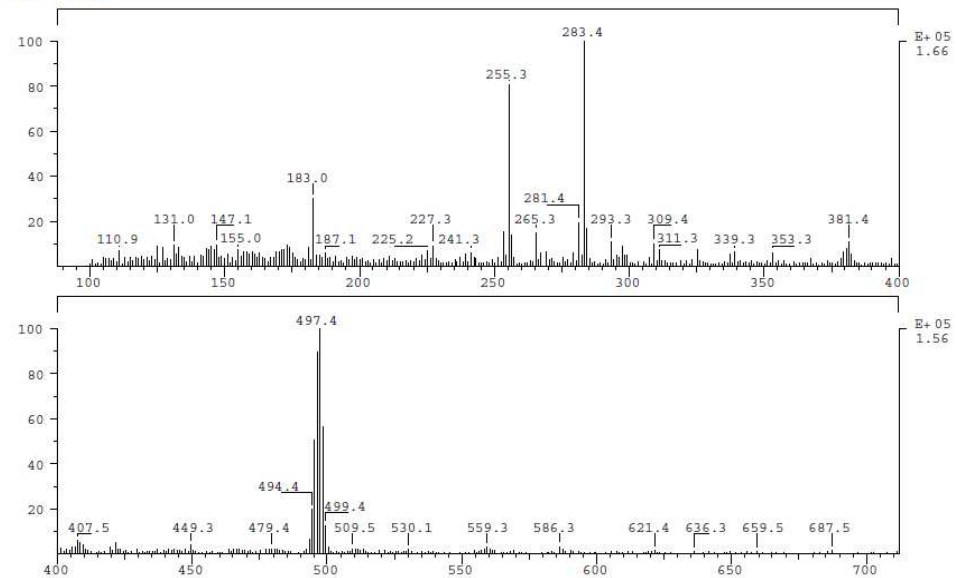


Figure S110. MS-FAB spectrum of compound **33**.

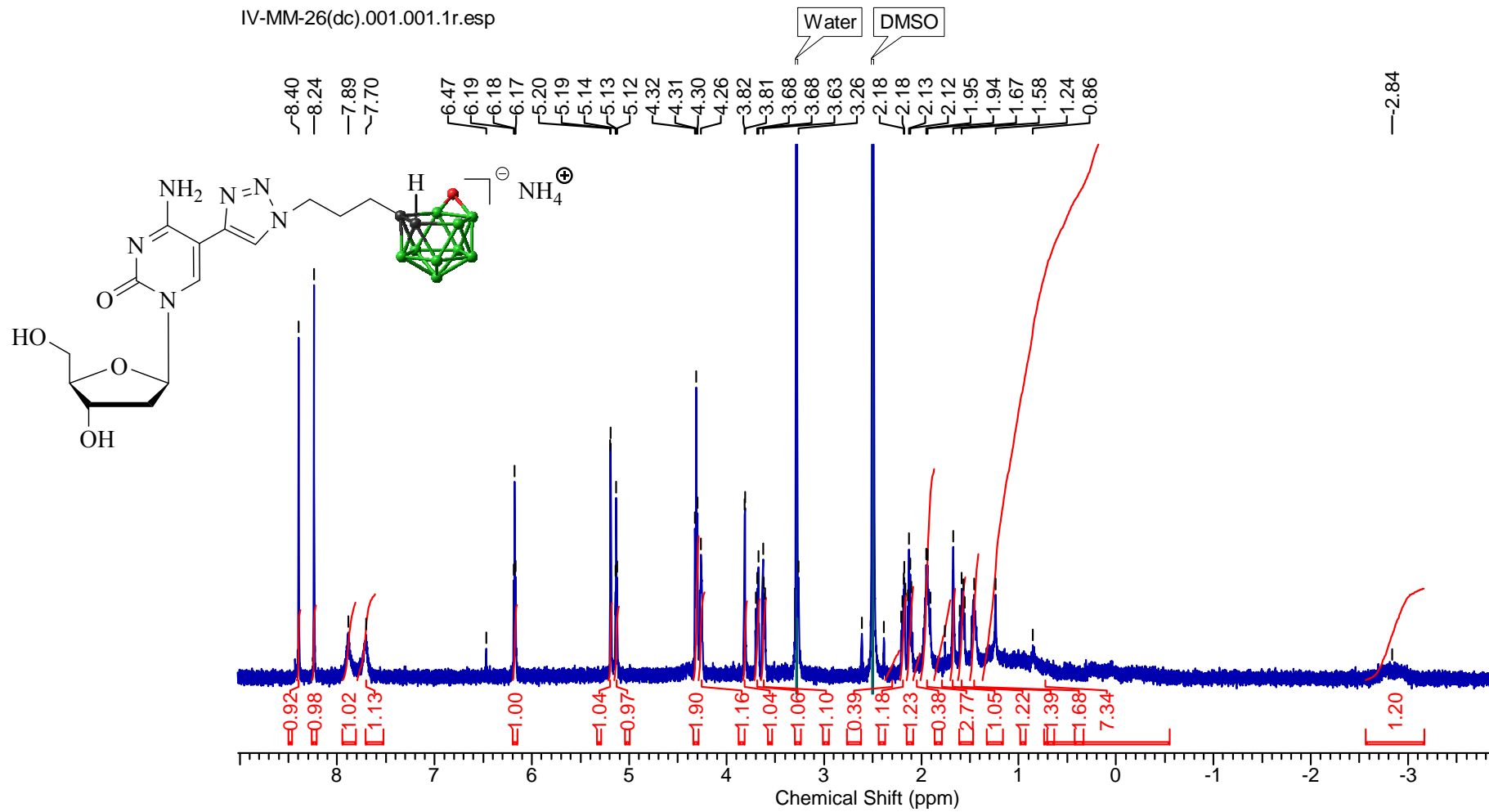


Figure S111. ^1H NMR spectrum of compound 34.

SPEC: az4661bm 23-Dec-13 REG : 00:16.9 #9
Samp: IV-MM-26 (DC) Start : 10:07:44 10
Comm: L51, Cs+ 13 keV, gly
Mode: FAB -VE -LMR ESCAN (EXP) UP LR NRM Study : MS CBM1M PAN Lodz
Oper: ew Client: IHM A.Olejniczak Inlet :
Base: 183.1 Inten : 3588431 Masses: 100 > 1127
Norm: 183.1 RIC : 22461523 #peaks: 999
Peak: 1000.00 mmu
Data: +1>10

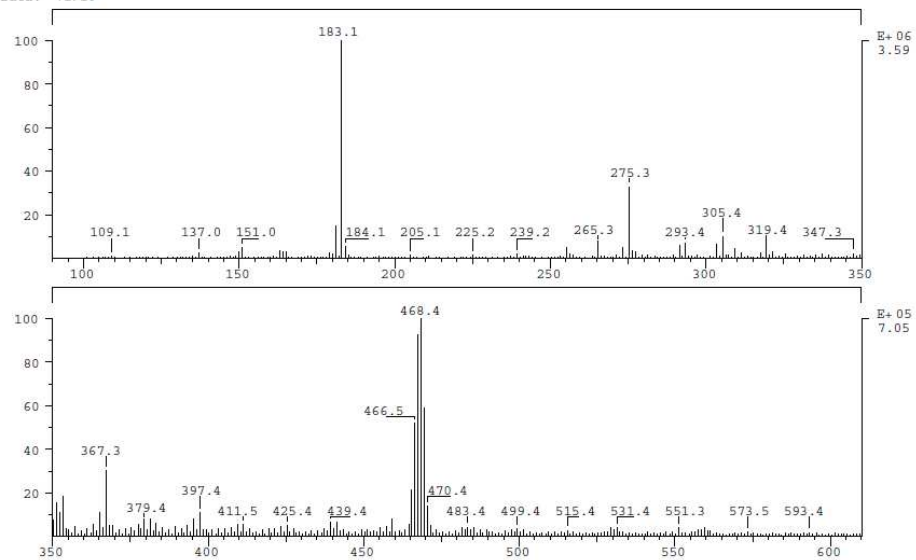


Figure S112. MS-FAB spectrum of compound **34**.

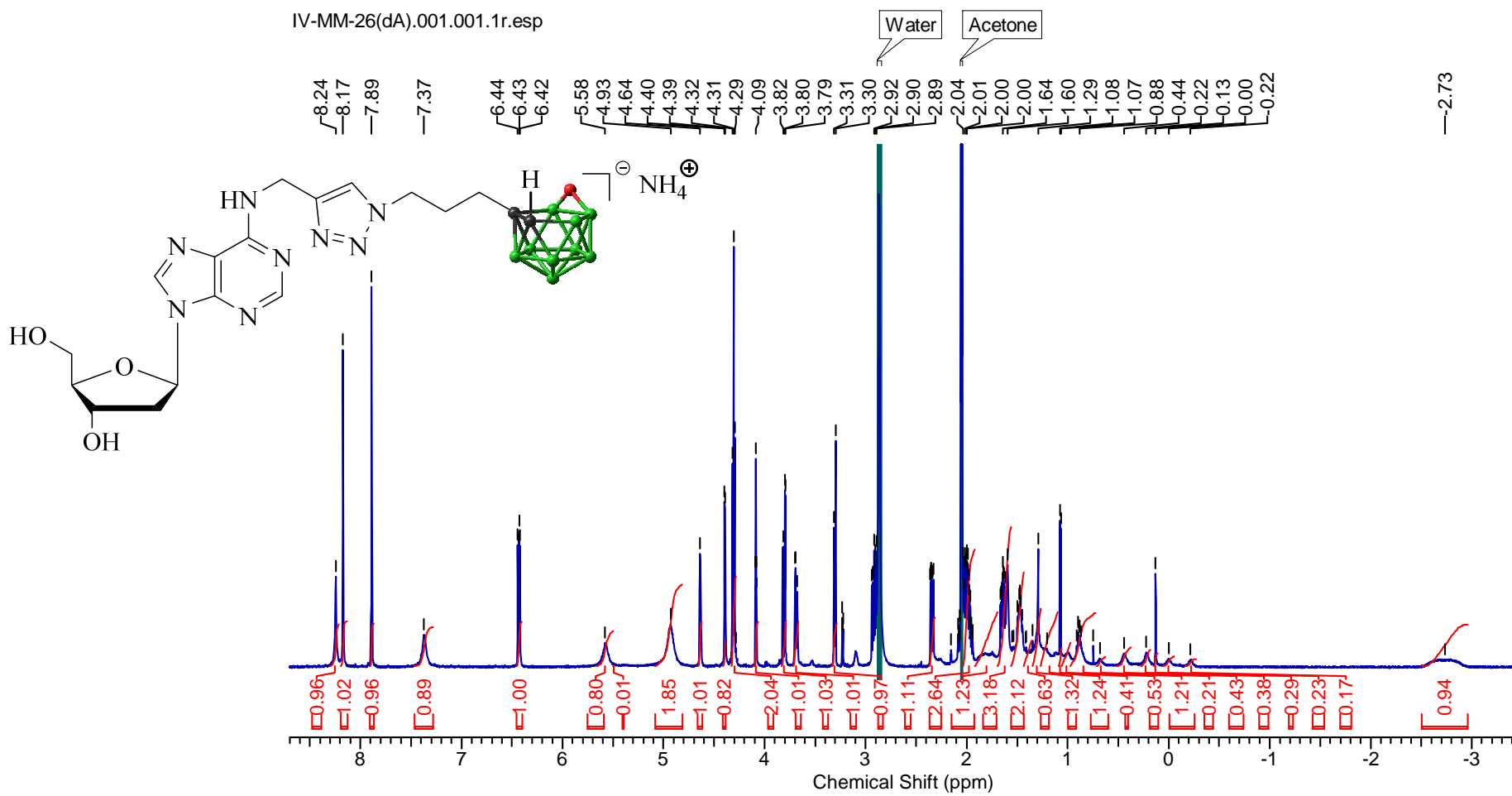


Figure S113. ^1H NMR spectrum of compound 35.

SPEC: ay3601bm_b 11-Jan-13 REG : 00:16.9 #9
Samp: dA-mido Start : 16:11:32 10
Comm: LSI, Cs+ 13 keV, gly
Mode: FAB -VE - +LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
Oper: ed Client: IBM PAN A.Olejnicza Inlet :
Base: 182.9 Inten : 63206 Masses: 100 > 1117
Norm: 182.9 RIC : 719303 #peaks: 467
Peak: 1000.00 mmu
Data: +1>10

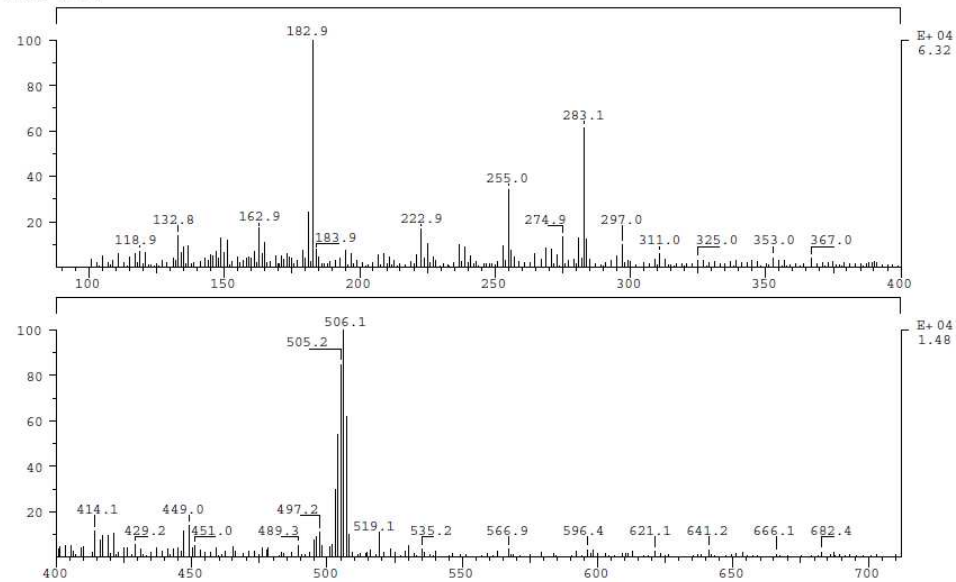
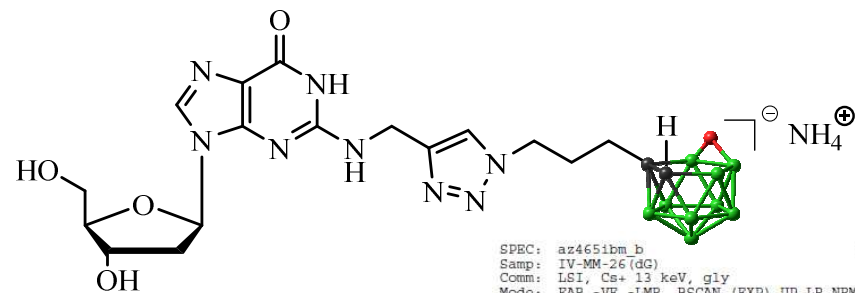


Figure S114. MS-FAB spectrum of compound **35**.



SPEC: az4651bm_b 23-Dec-13 REG : 00:16.9 #9
 Samp: IV-MM-26(dG) Start : 09:43:28 10
 Comm: LSI, Cs+ 13 keV, gly
 Mode: FAB -VE -LMR BSCAN (EXP) UP LR NRM Study : MS CBMIM PAN Lodz
 Oper: ew Client: IBM A.Olejniczak Inlet :
 Base: 265.3 Inten : 765038 Masses: 100 > 1127
 Norm: 265.3 RIC : 16512061 #peaks: 1000
 Peak: 1000.00 mmu
 Data: +1>10

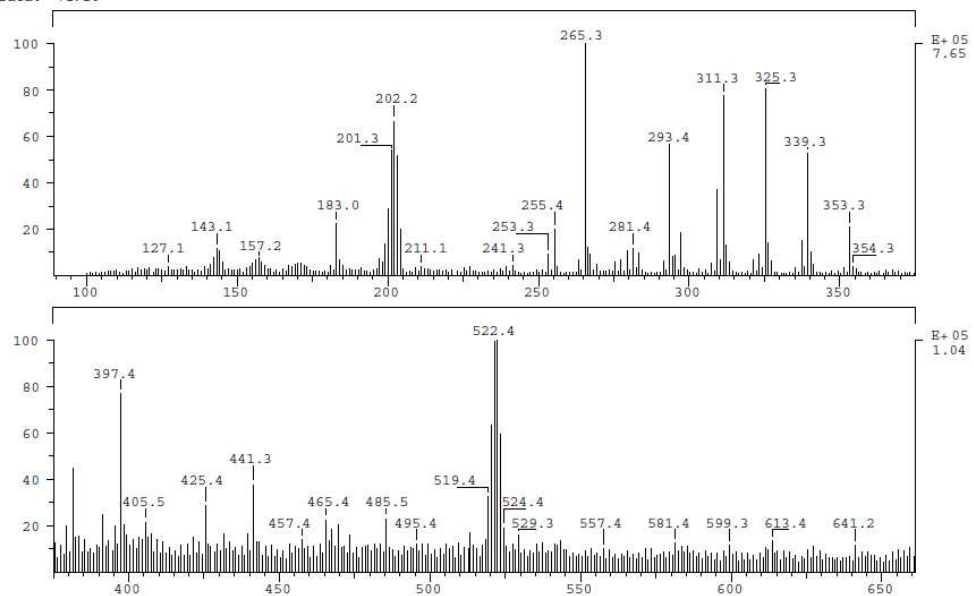


Figure S115. MS-FAB spectrum of compound **36**.

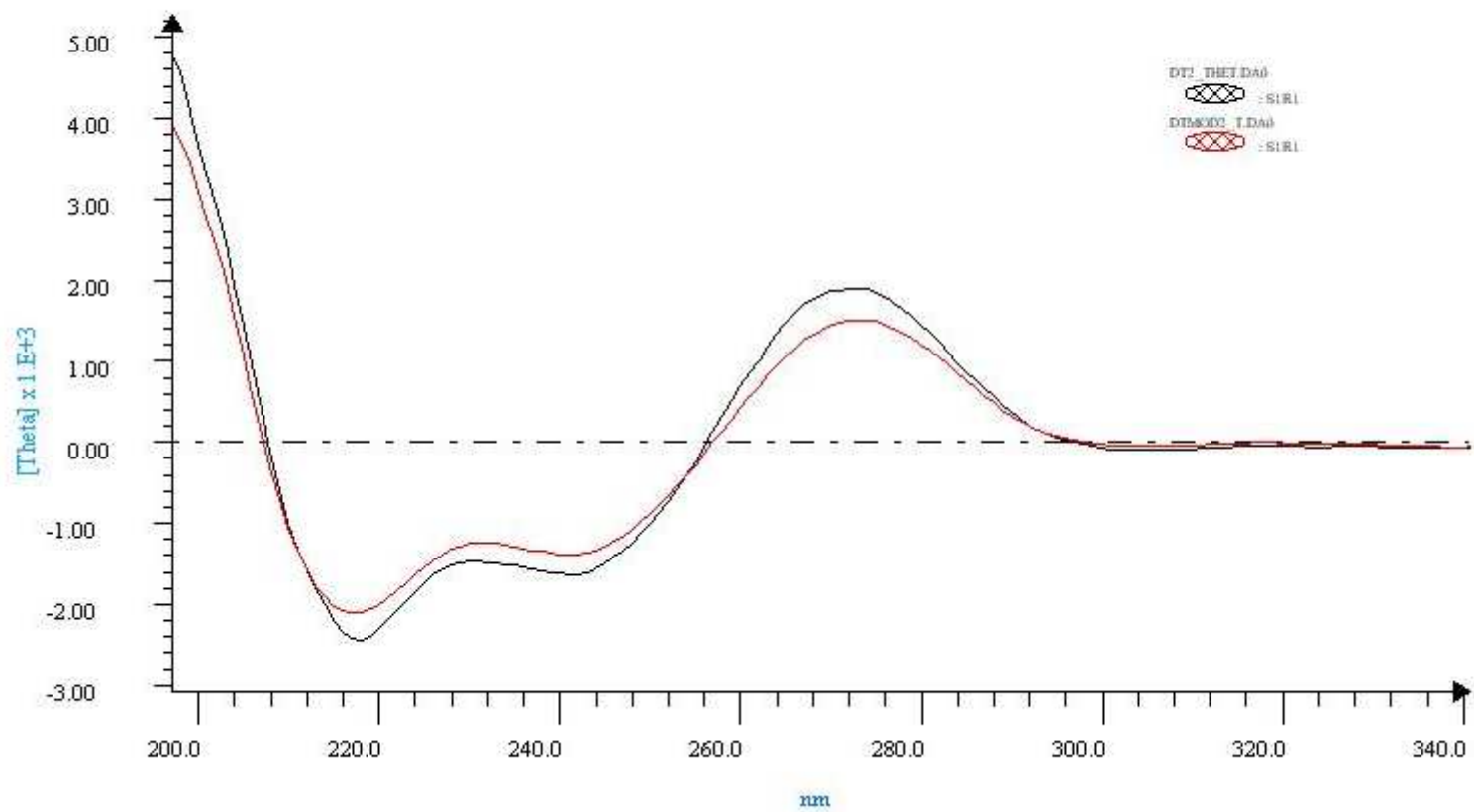


Figure S116. CD spectra of compounds **20** (red) and thymidine (black).

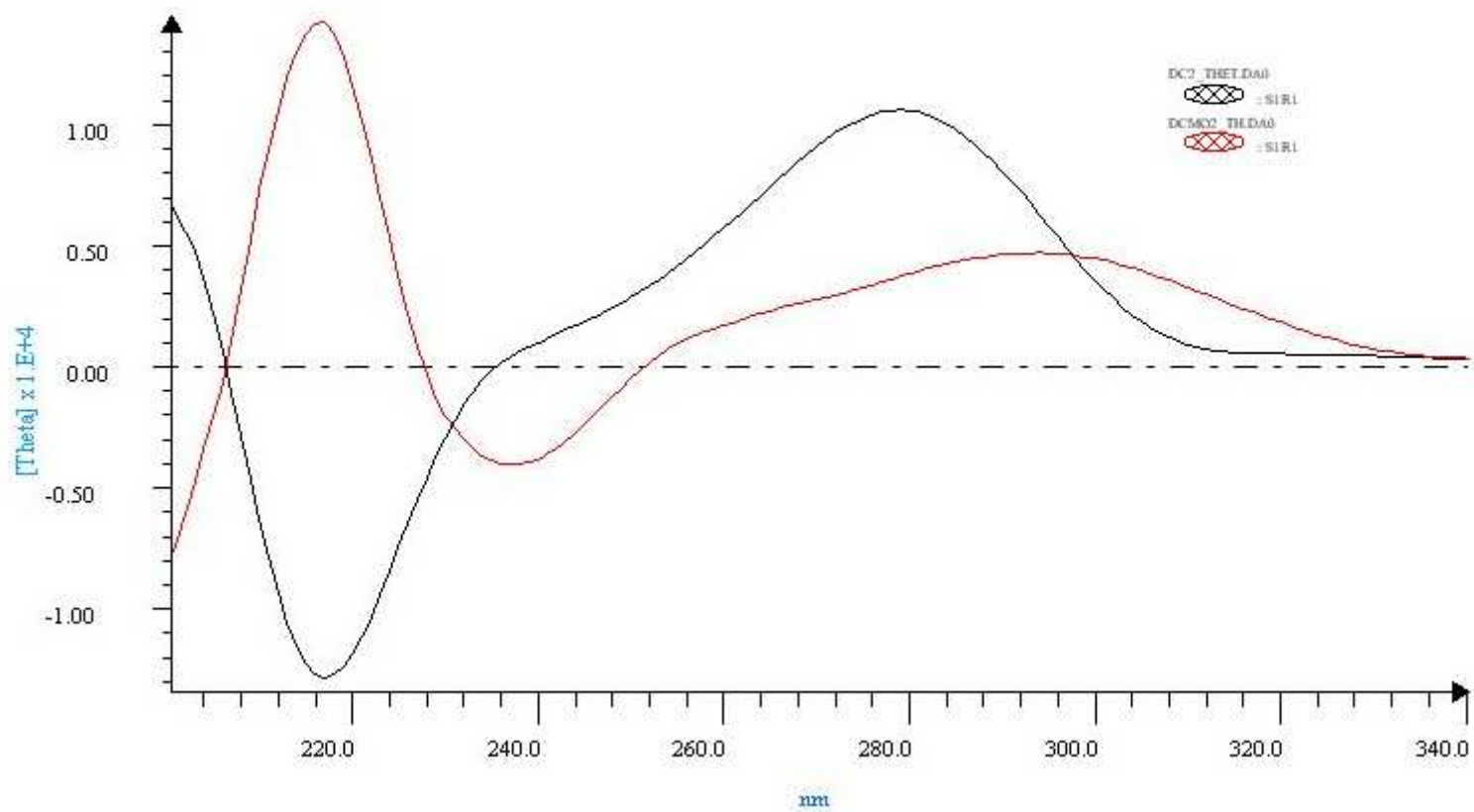


Figure S117. CD spectra of compounds **22** (red) and 2'-deoxycytidine (black).

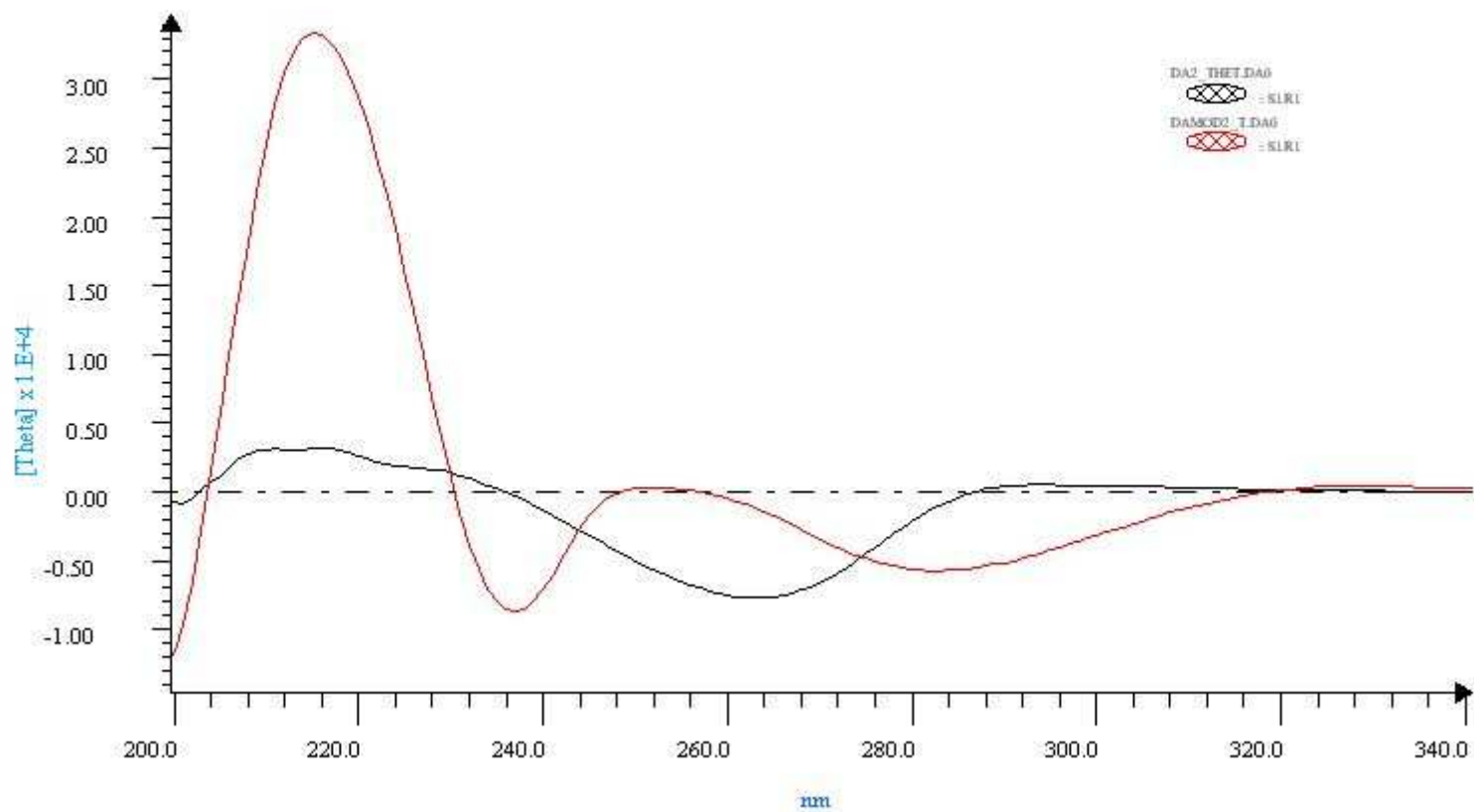


Figure S118. CD spectra of compounds **24** (red) and 2'-deoxyadenosine (black).

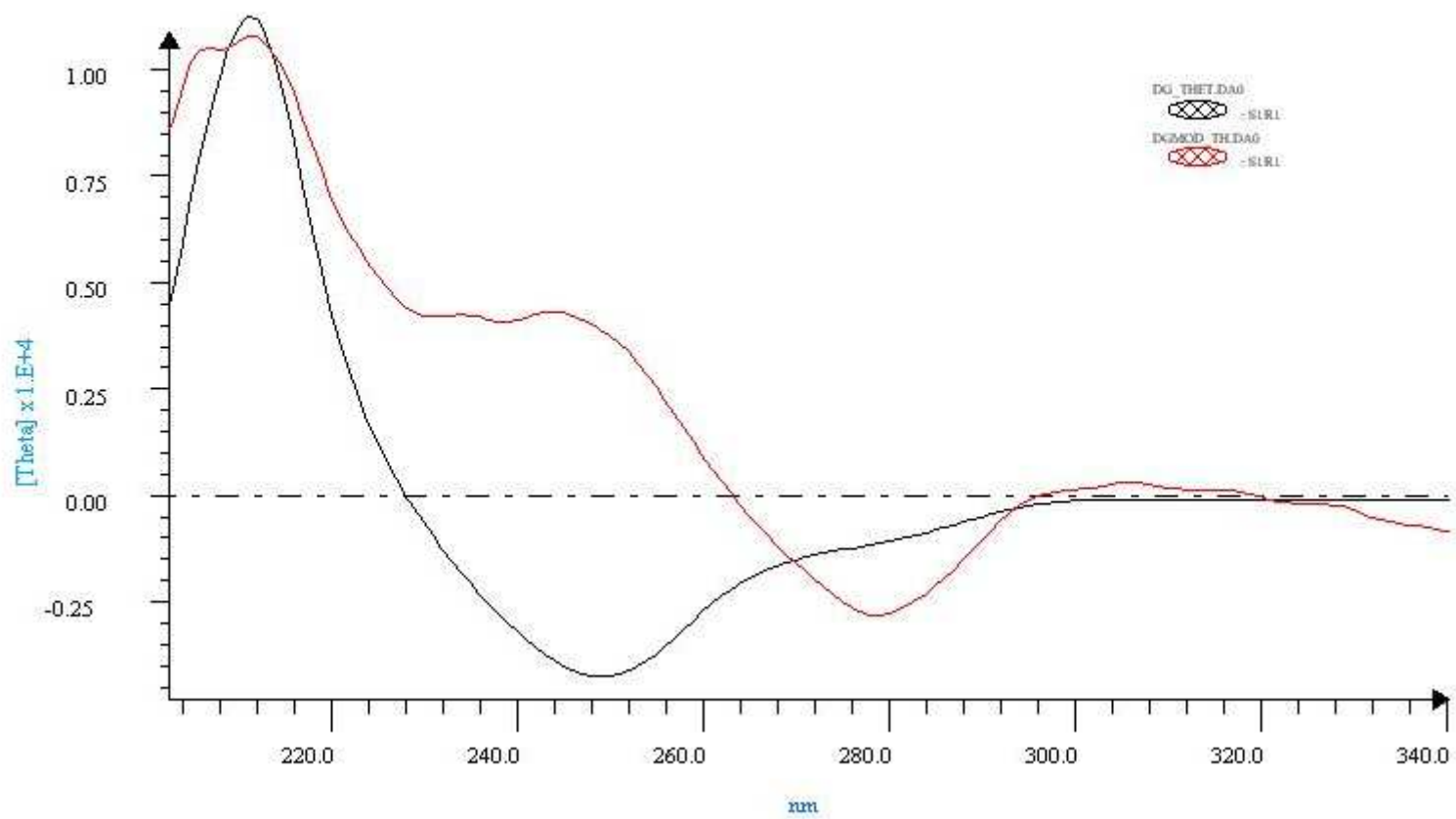
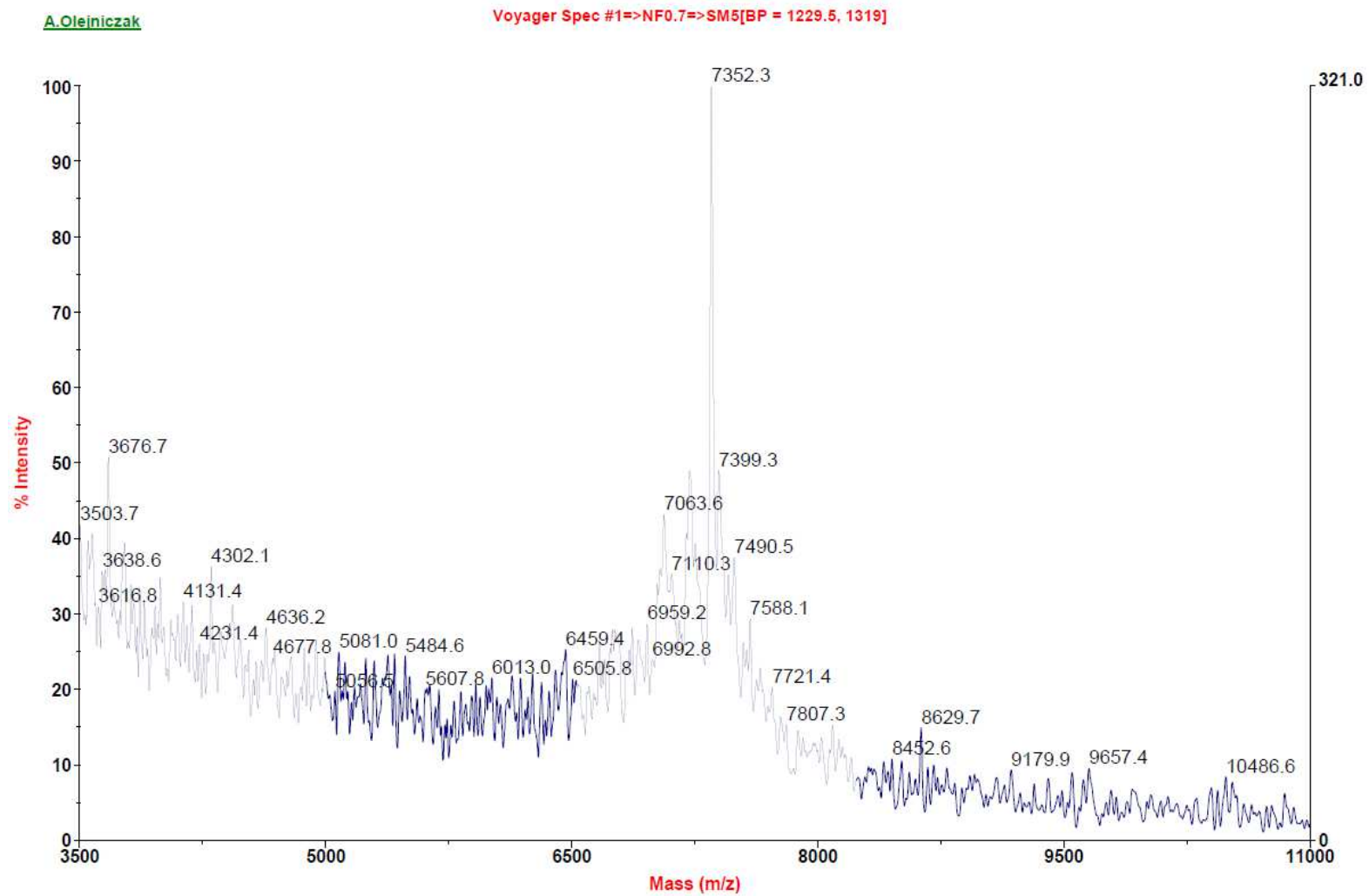
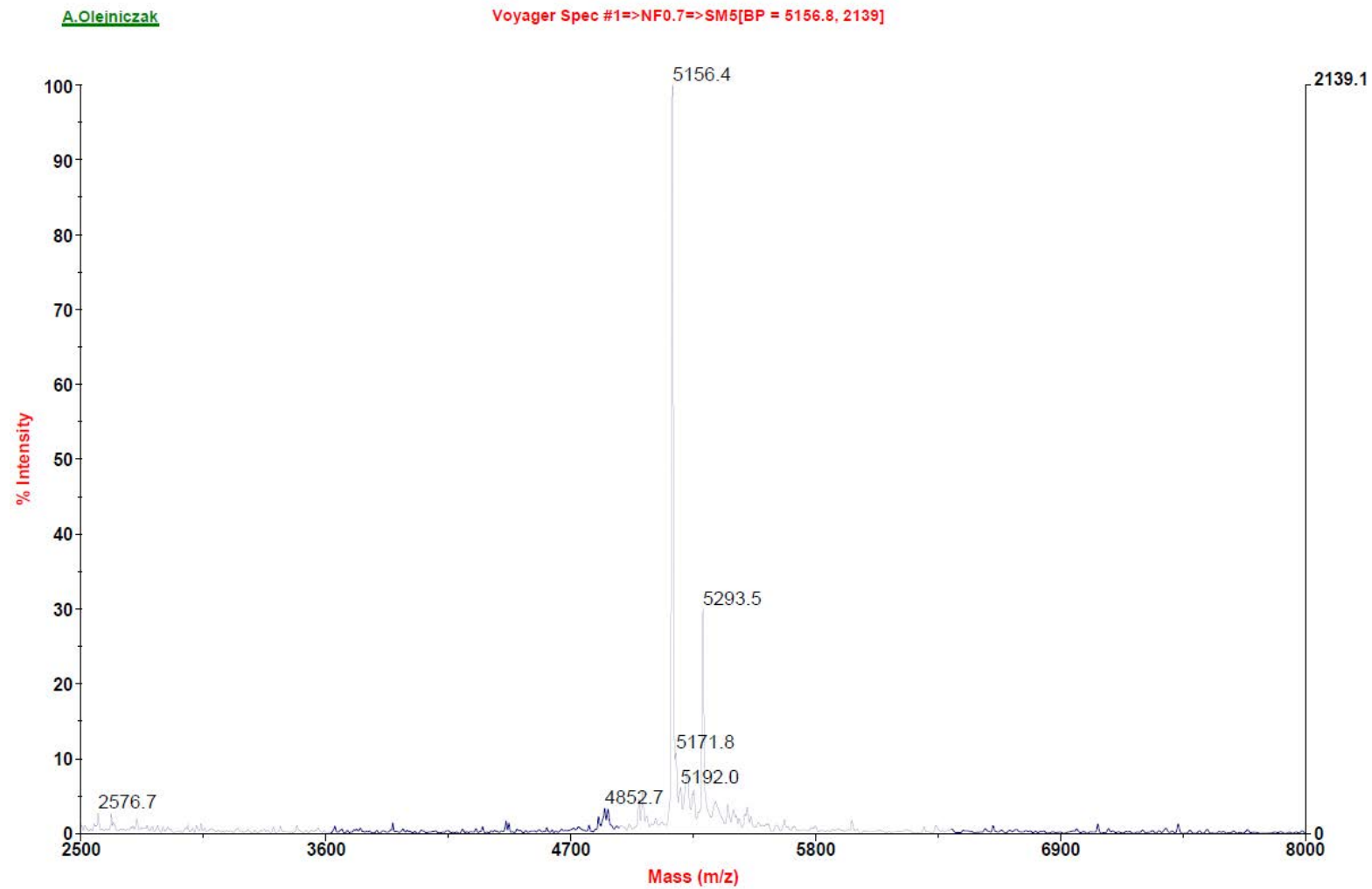


Figure S119. CD spectra of compounds **27** (red) and 2'-deoxyguanosine (black).



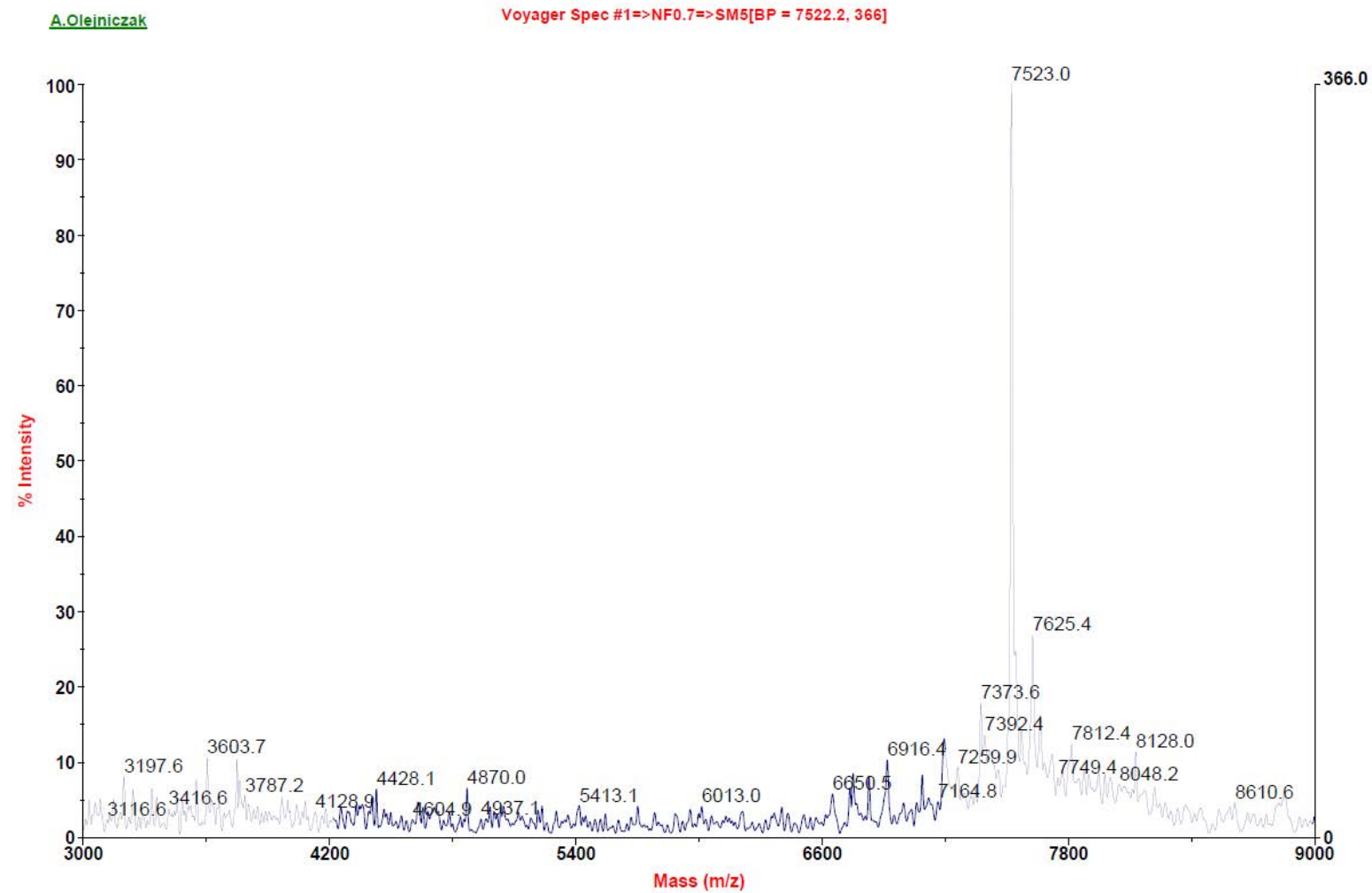
A.Olejniczak, XXXXI-AO-55, 0.01 OD (ACN/H₂O 1:1), IE, [HPA, 3-hydroxypicolinic acid, 50 mg/mL in 50% ACN/H₂O / AC, ammonium citrate dibasic, 50 mg/mL in H₂O]
 E:\...fg330011.dat
 Acquired: 15:16:00, October 11, 2013

Figure S120. MALDI-TOF spectrum of oligonucleotide **38**.



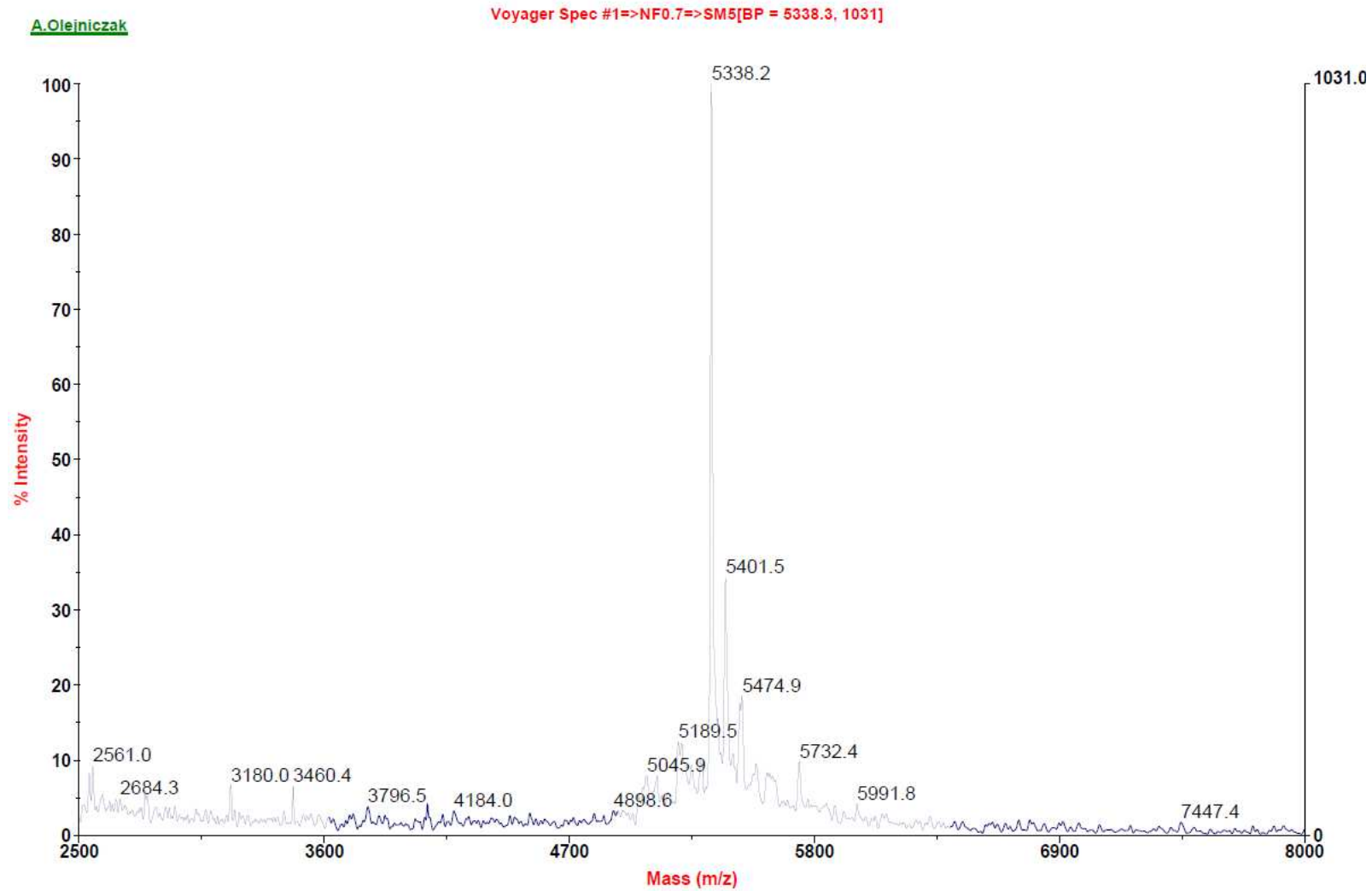
A.Olejniczak, XXXXI-AO-36, 0,01 OD (ACN/H2O 1:1), [HPA, 3-hydroxypicolinic acid, 50 mg/mL in 50% ACN/H2O / AC, ammonium citrate dibasic, 50 mg/mL in H2O - 8:1 (v/v)]
E:\...ff910001.dat
Acquired: 12:21:00, October 02, 2013

Figure S121. MALDI-TOF spectrum of oligonucleotide **39**.



A.Olejniczak, XXXXI-AO-95, 0,01 OD (ACN/H2O 1:1),[HPA, 3-hydroxypicolinic acid, 50 mg/mL in 50% ACN/H2O / AC, ammonium citrate dibasic, 50 mg/mL in H2O - 8:1 (v/v)]
 E:\...fh850001.dat
 Acquired: 13:53:00, December 18, 2013

Figure S122. MALDI-TOF spectrum of oligonucleotide **40**.



A.Olejniczak, XXXXI-AO-77, 0,01 OD (ACN/H₂O 1:1), [HPA, 3-hydroxypicolinic acid, 50 mg/mL in 50% ACN/H₂O / AC, ammonium citrate dibasic, 50 mg/mL in H₂O - 8:1 (v/v)]
E:\...fg640004.dat
Acquired: 13:16:00, November 05, 2013

Figure S123. MALDI-TOF spectrum of oligonucleotide **41**.