

SUPPLEMENTARY MATERIALS

Biological activity evaluation of phenolic isatin-3-hydrazones containing a quaternary ammonium center of various structures

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Contents

Copies of NMR spectra	2-73
Copies of IR spectra	74-86
Copies of mass-spectra	87-112

Copies of NMR spectra

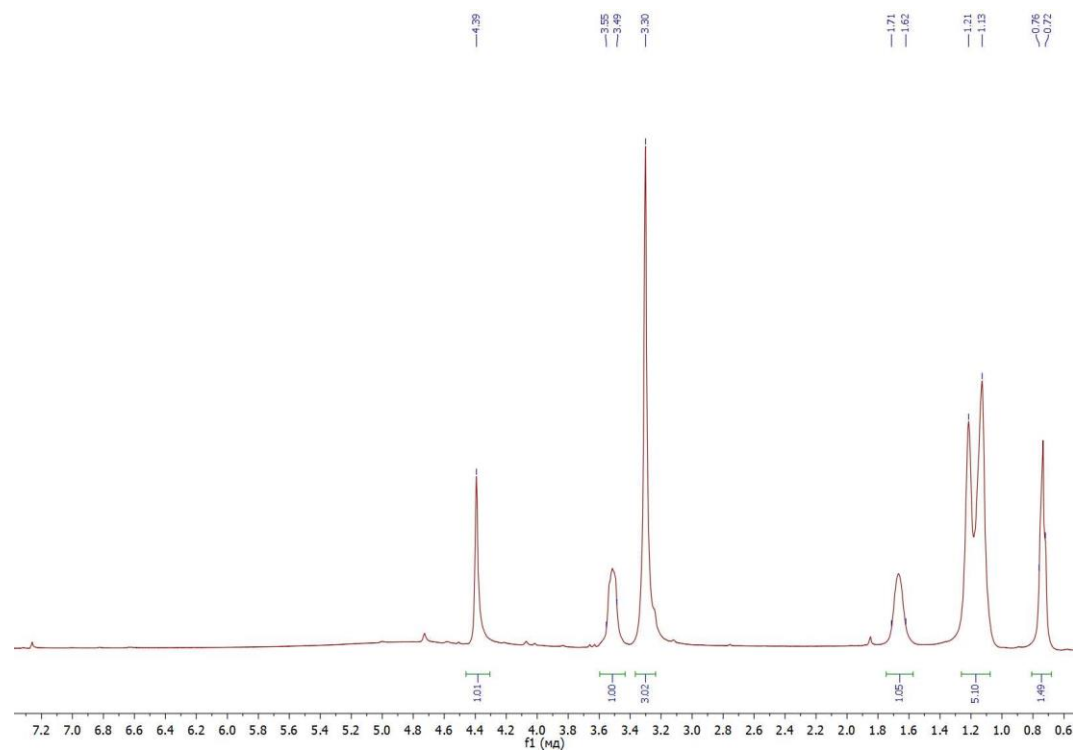


Figure S1. ^1H NMR spectrum of compound **1a** (400 MHz, CDCl_3)

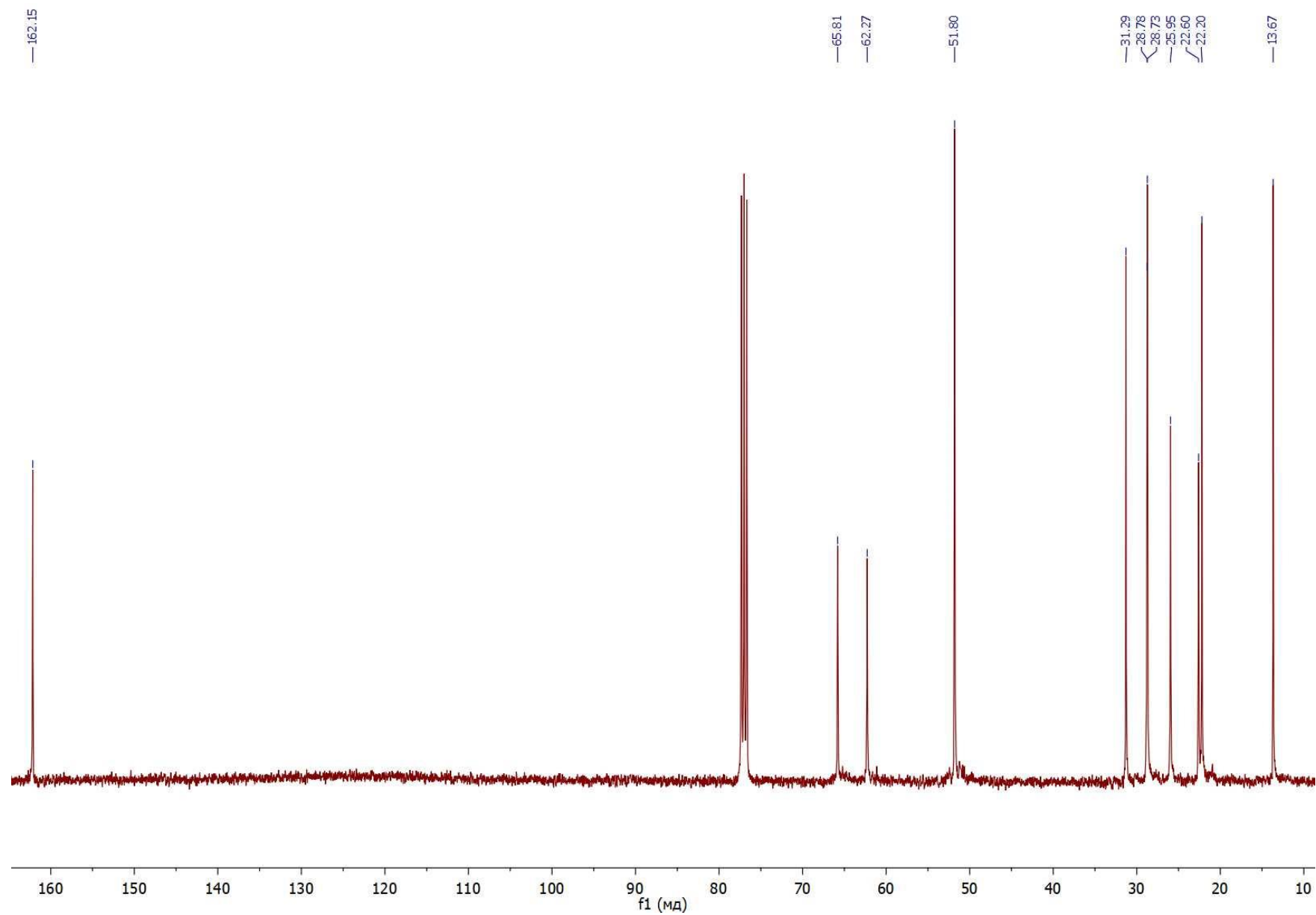


Figure S2. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **1a** (101 MHz, CDCl_3)

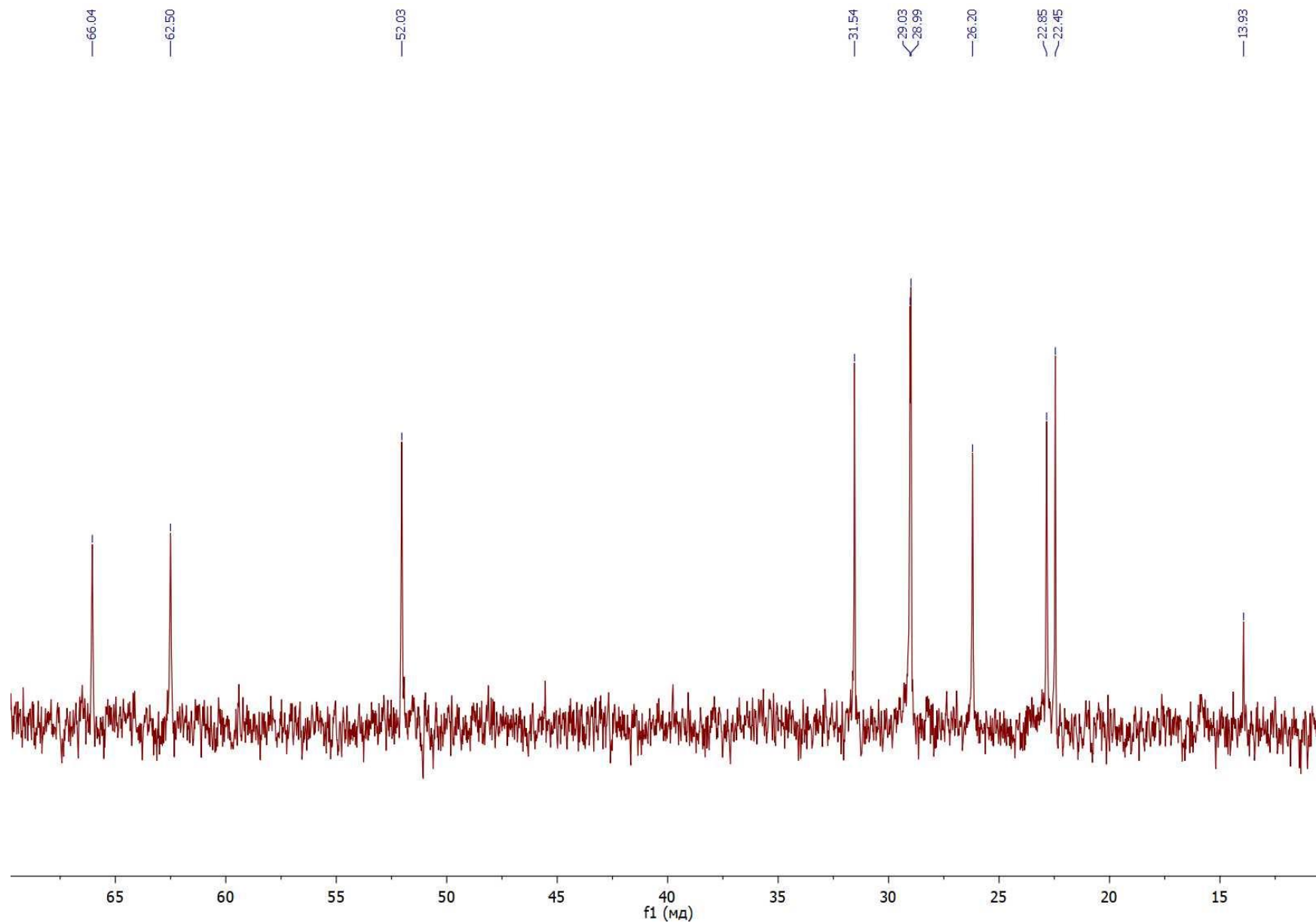


Figure S3. ^{13}C (dept) NMR spectrum of compound **1a** (101 MHz, CDCl_3)

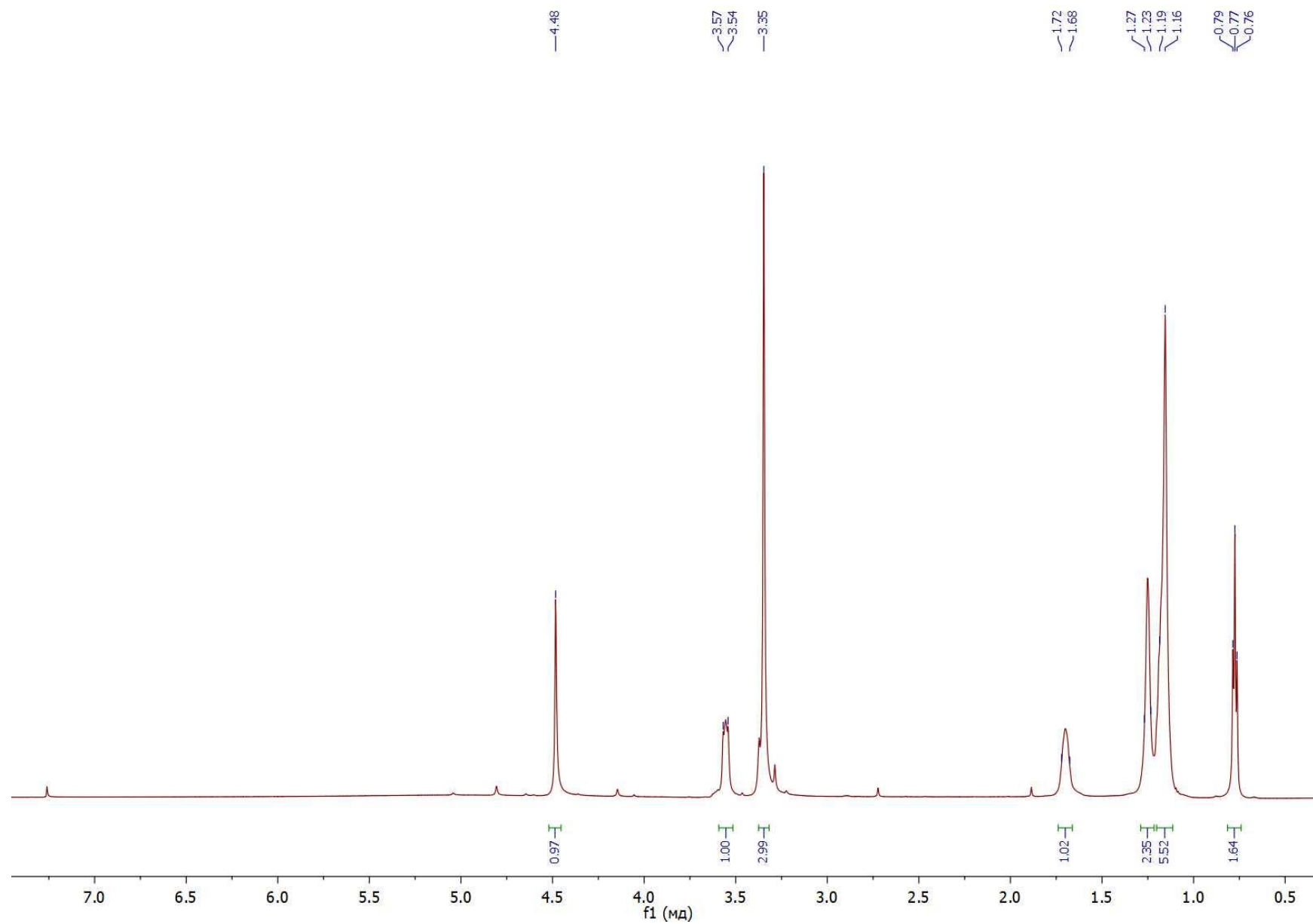


Figure S4. ¹H NMR spectrum of compound **1b** (600 MHz, CDCl₃)

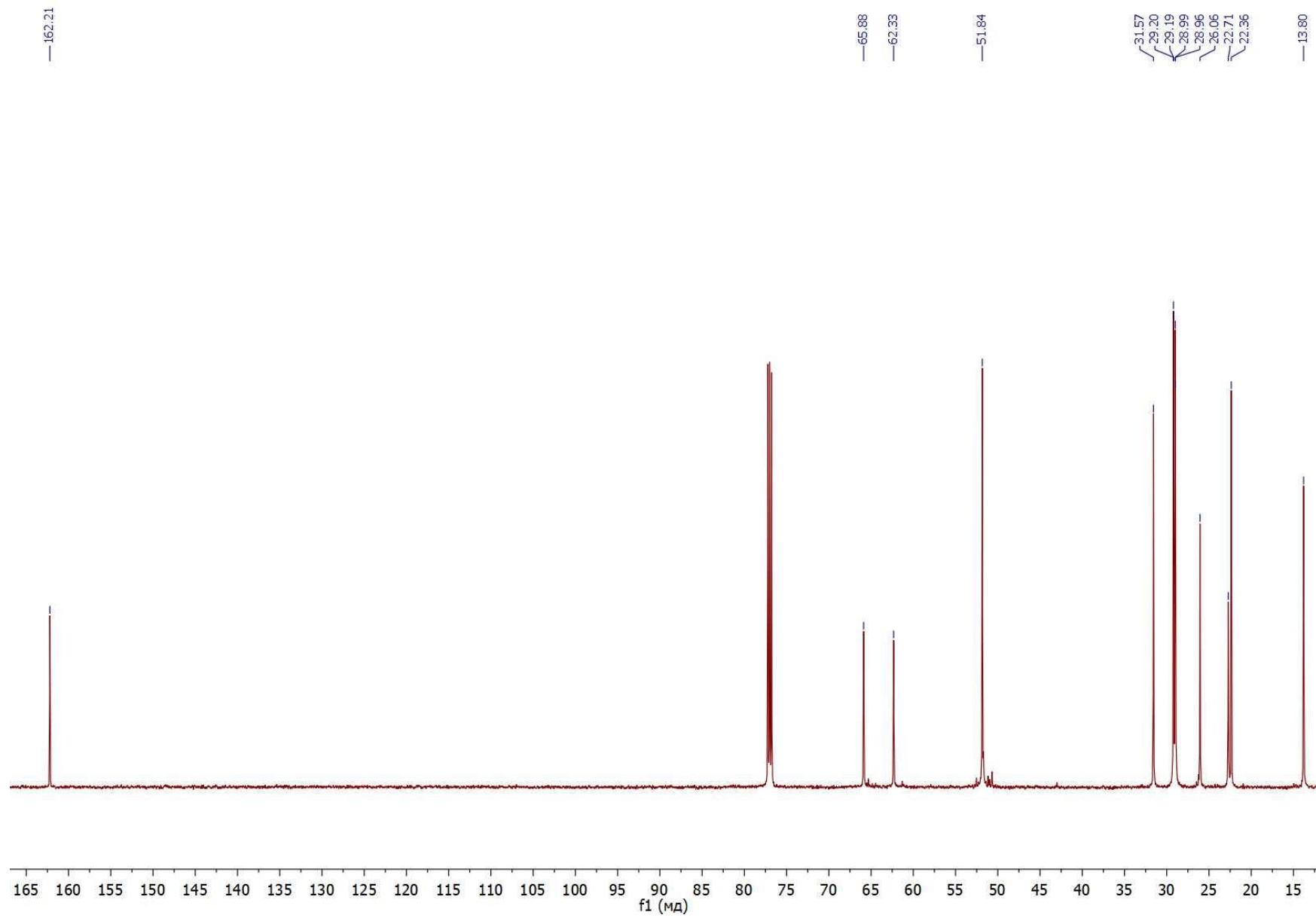


Figure S5. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **1b** (151 MHz, CDCl_3)

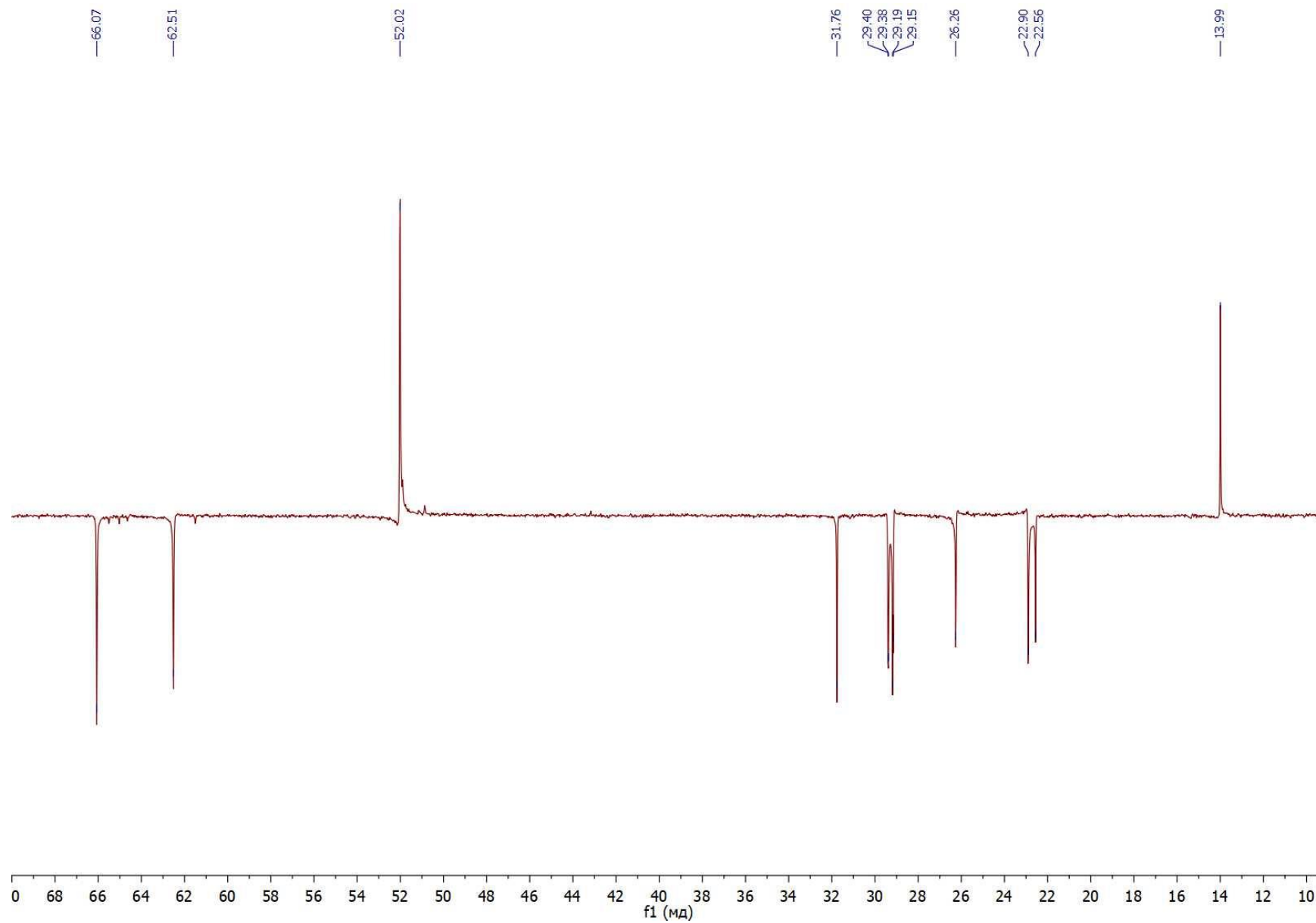


Figure S6. ^{13}C (dept) NMR spectrum of compound **1b** (151 MHz, CDCl_3)

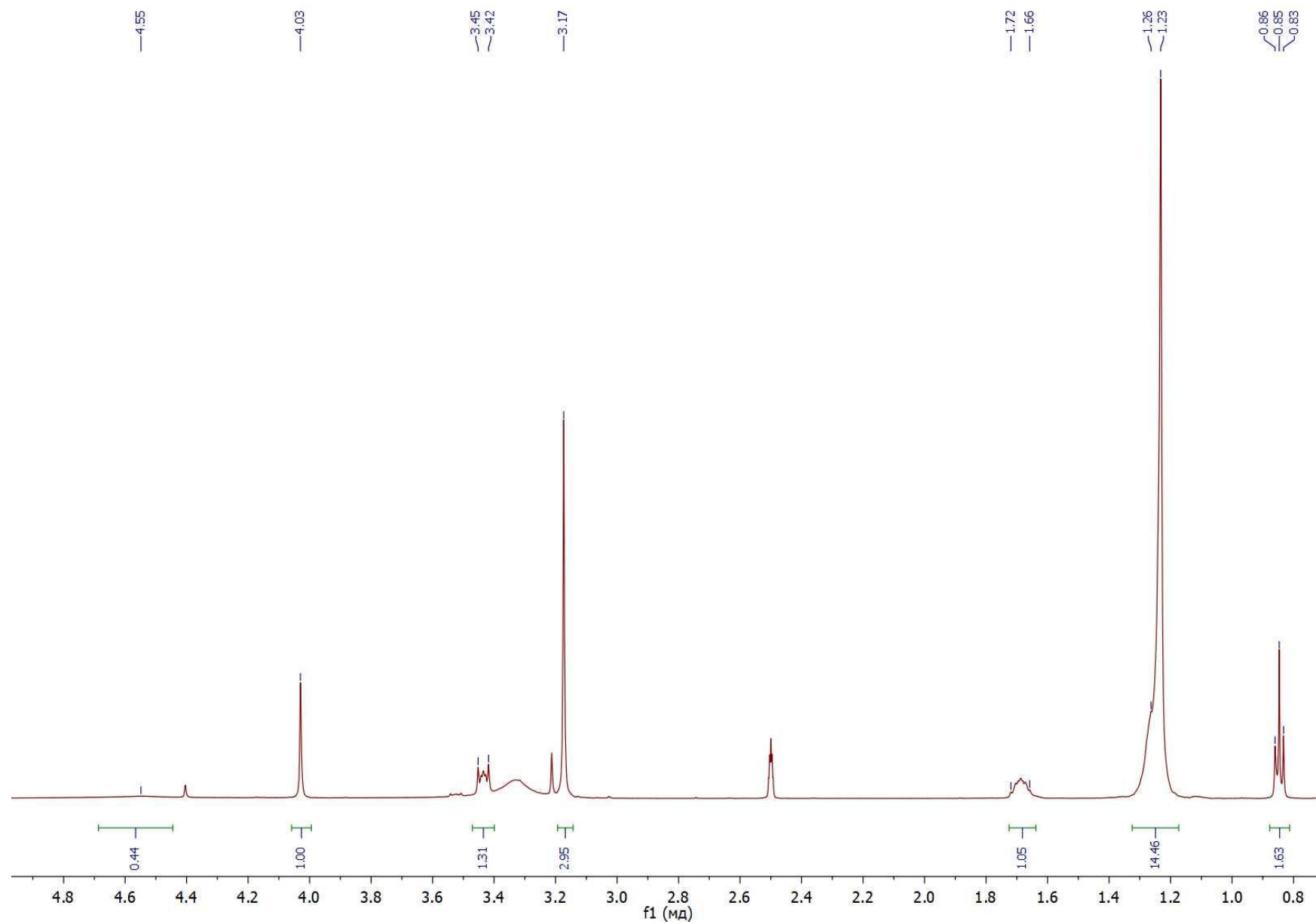


Figure S7. ¹H NMR spectrum of compound **1c** (400 MHz, DMSO-*d*₆)

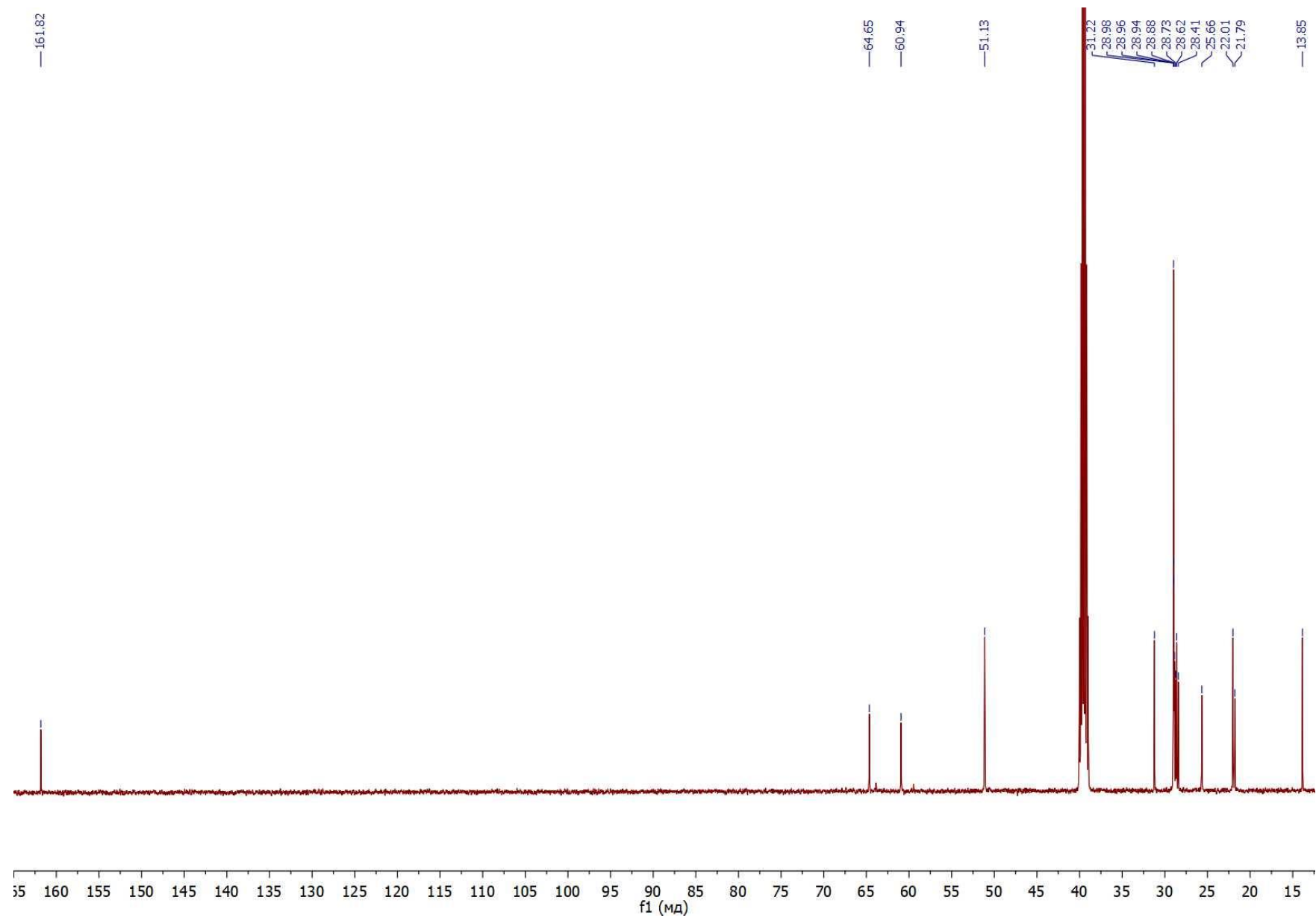


Figure S8. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **1c** (101 MHz, $\text{DMSO}-d_6$)

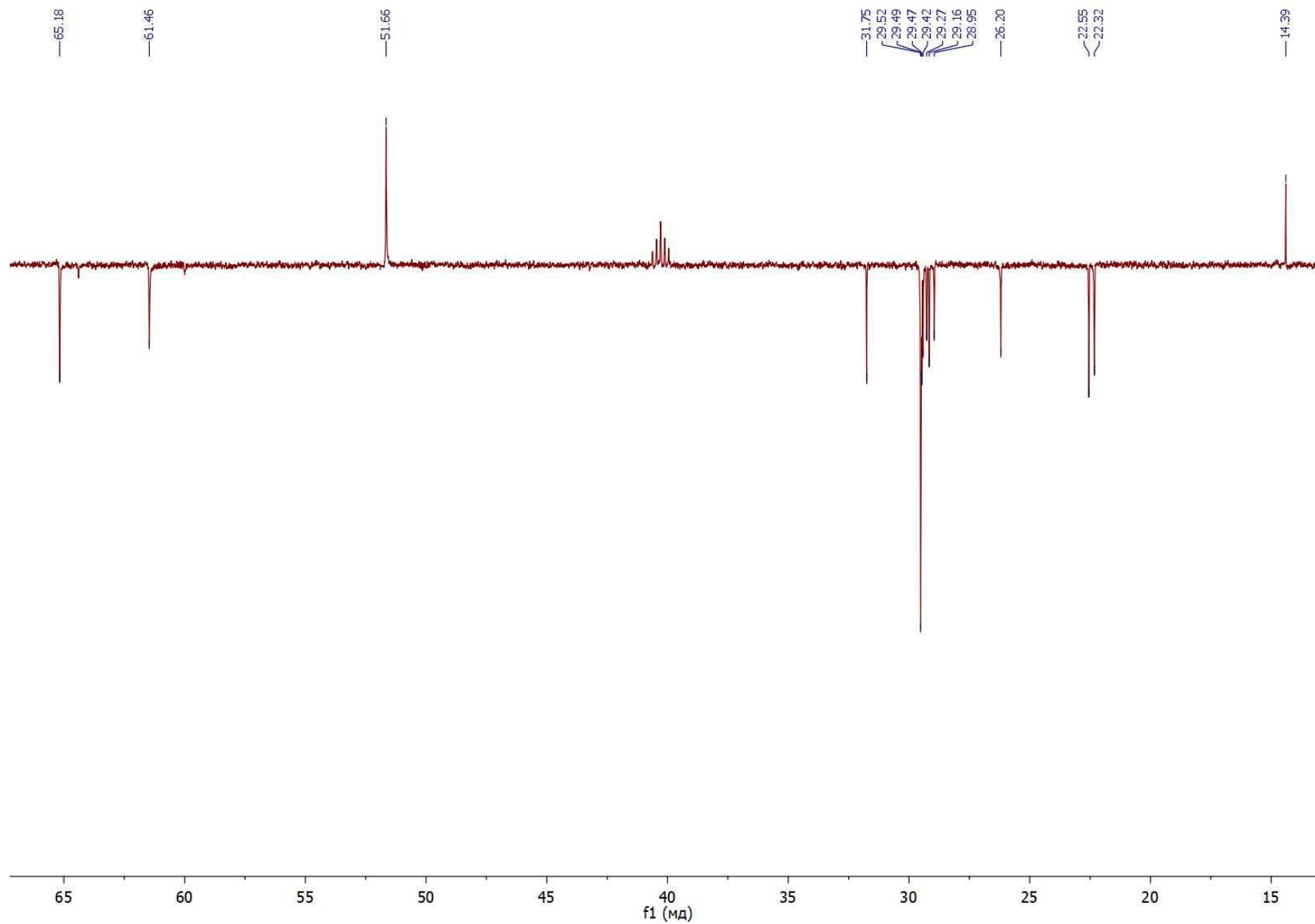


Figure S9. ^{13}C (dept) NMR spectrum of compound **1c** (101 MHz, DMSO- d_6)

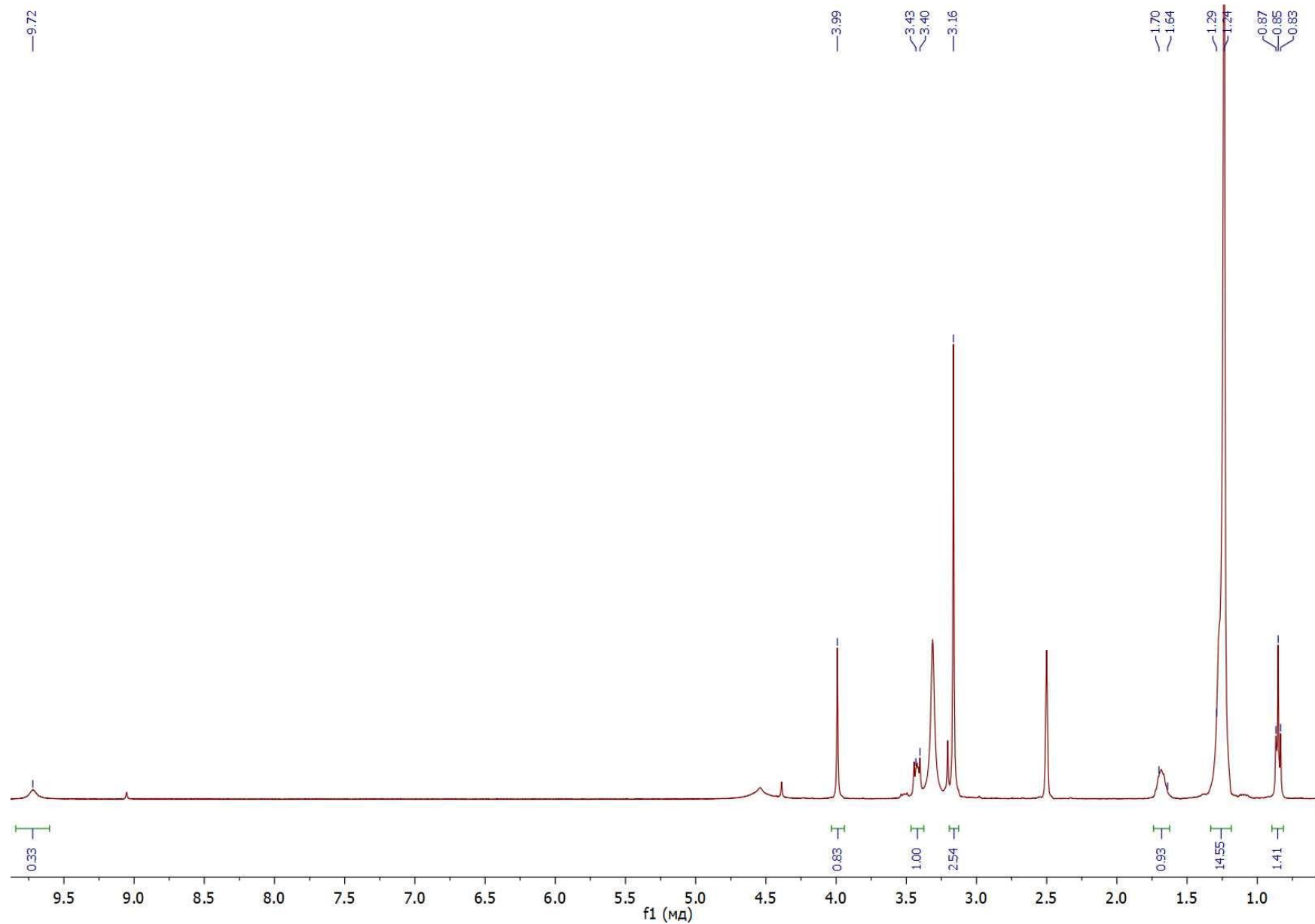


Figure S10. ¹H NMR spectrum of compound **1d** (400 MHz, DMSO-*d*₆)

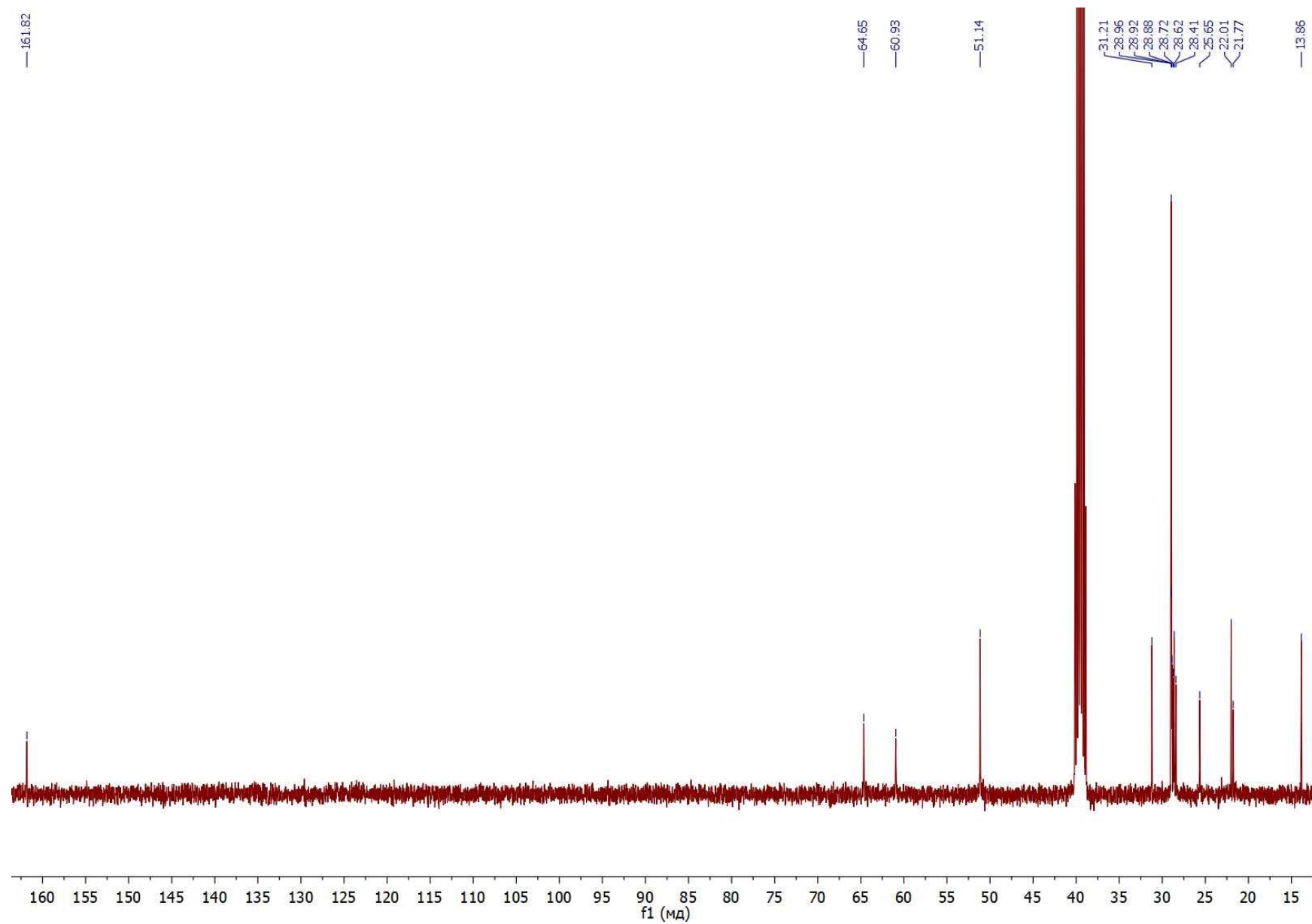


Figure S11. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **1d** (101 MHz, DMSO- d_6)

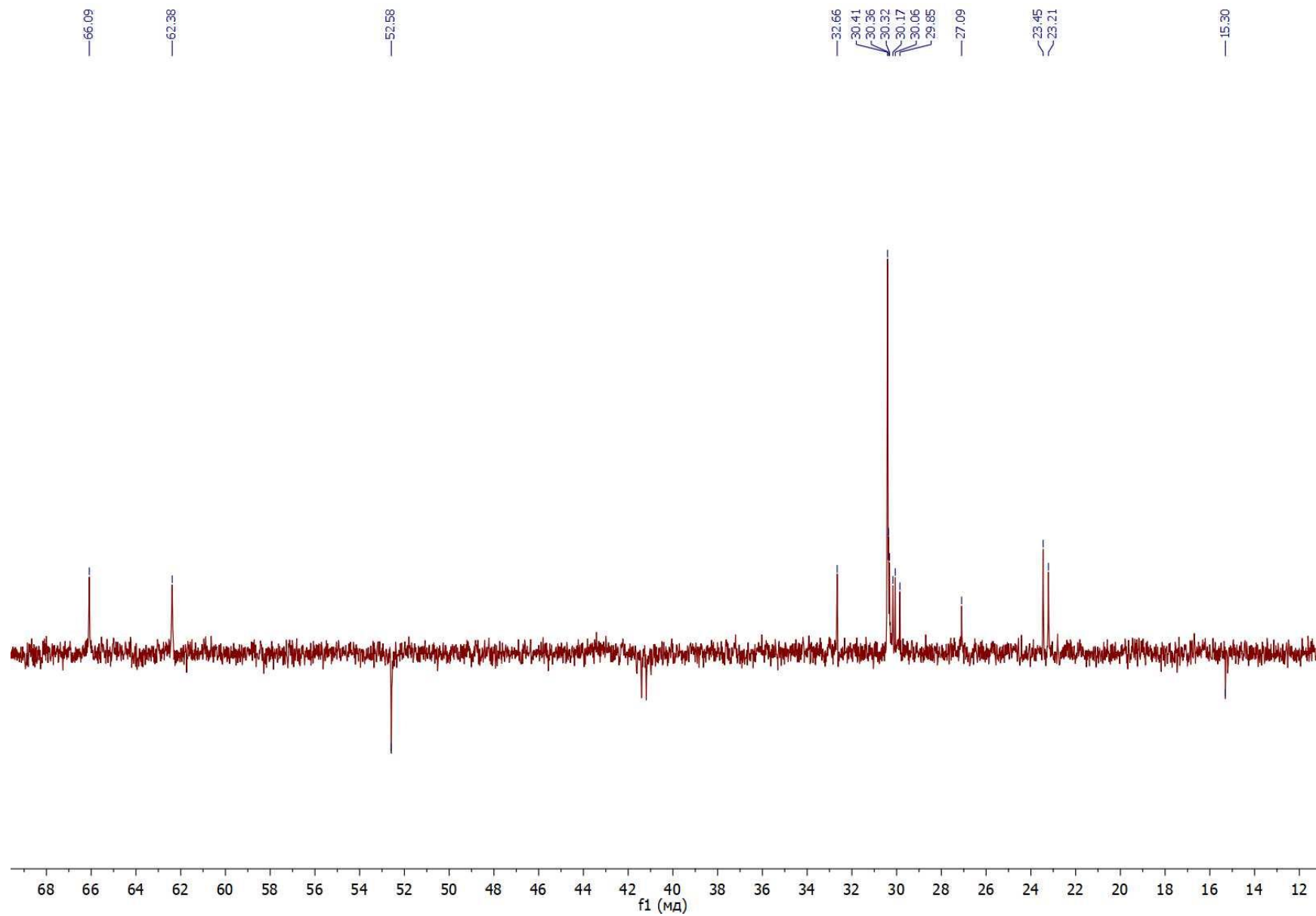


Figure S12. ^{13}C (dept) NMR spectrum of compound **1d** (101 MHz, $\text{DMSO-}d_6$)

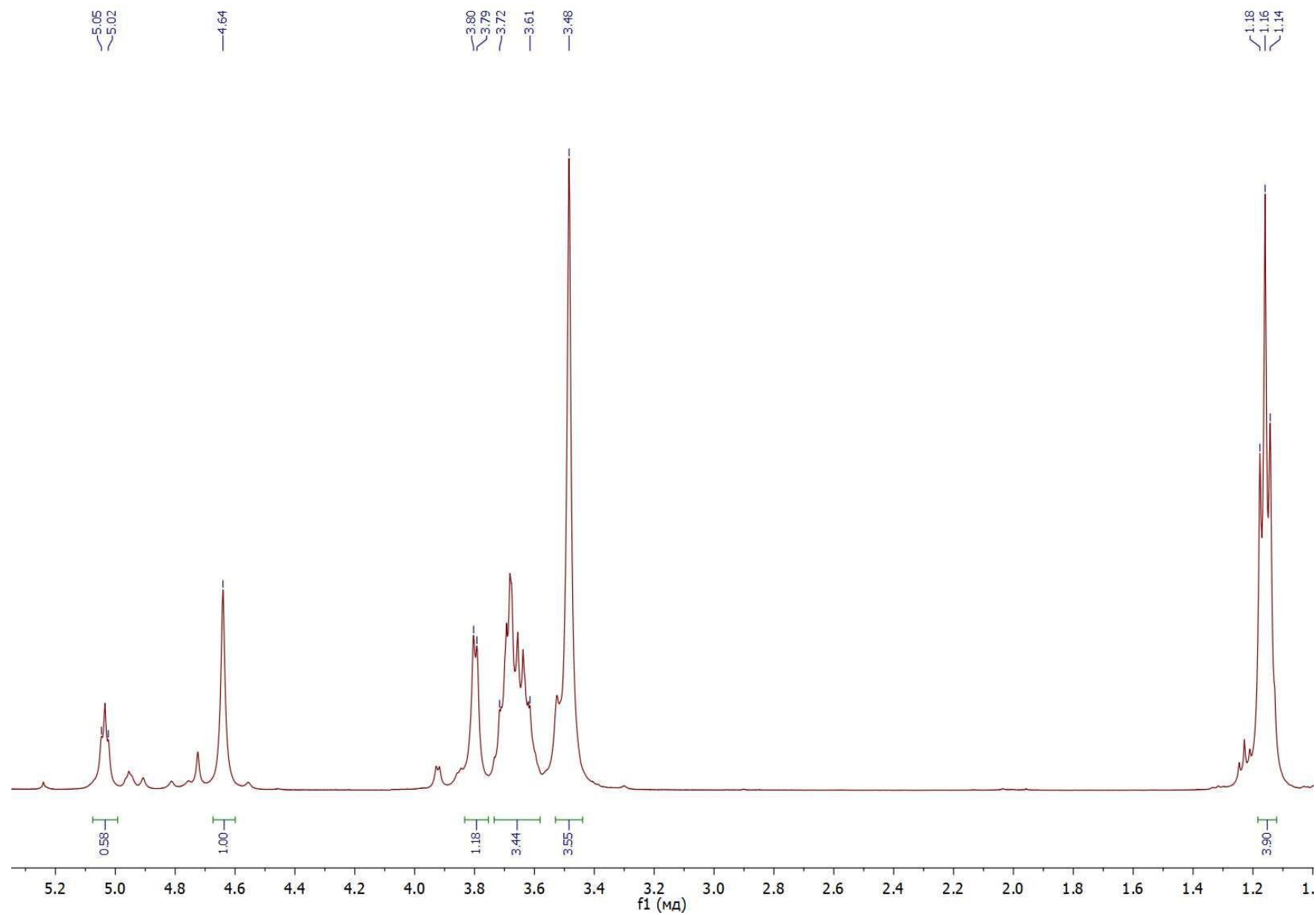


Figure S13. ^1H NMR spectrum of compound **1e** (400 MHz, CDCl_3)

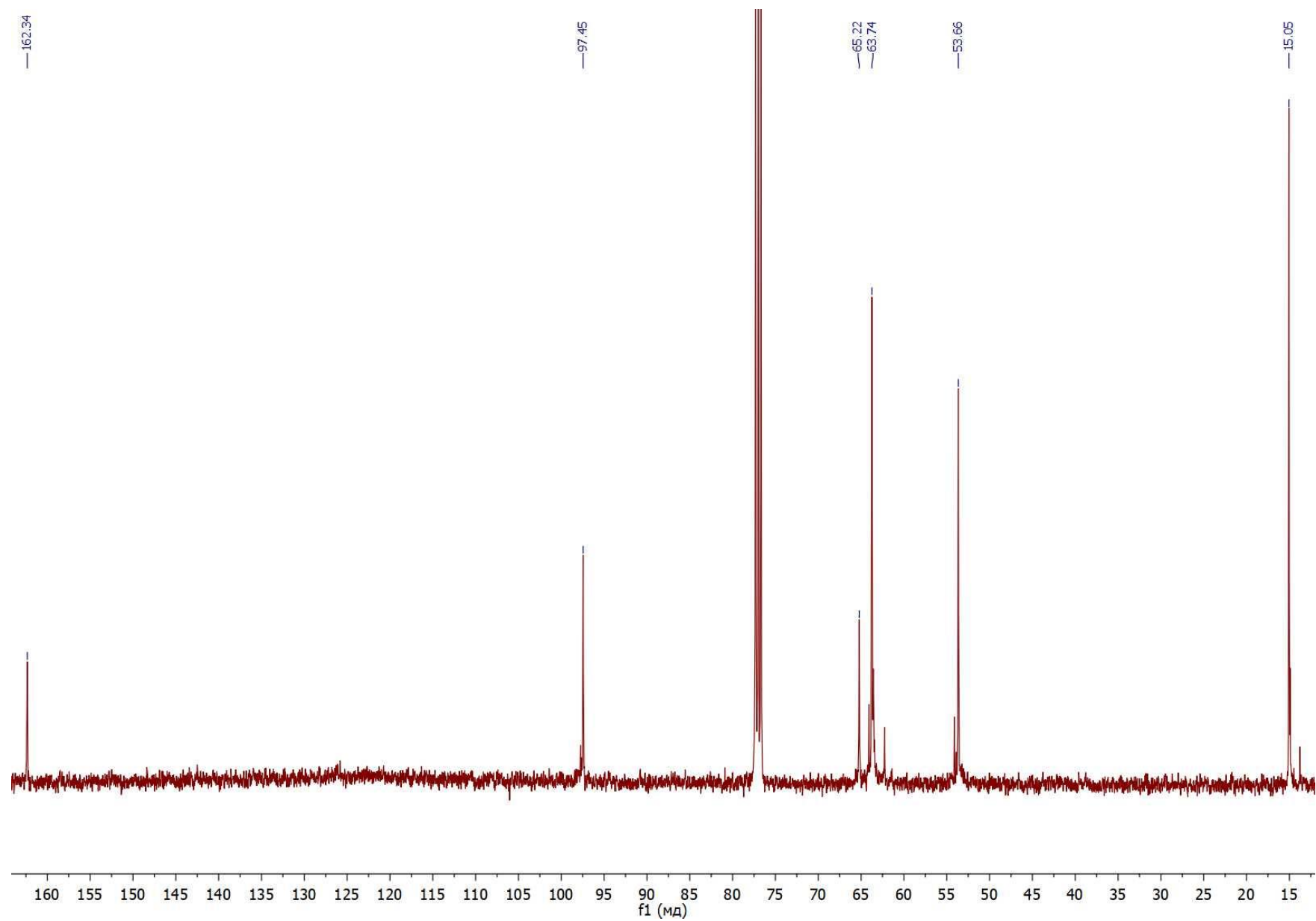


Figure S14. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **1e** (101 MHz, CDCl_3)

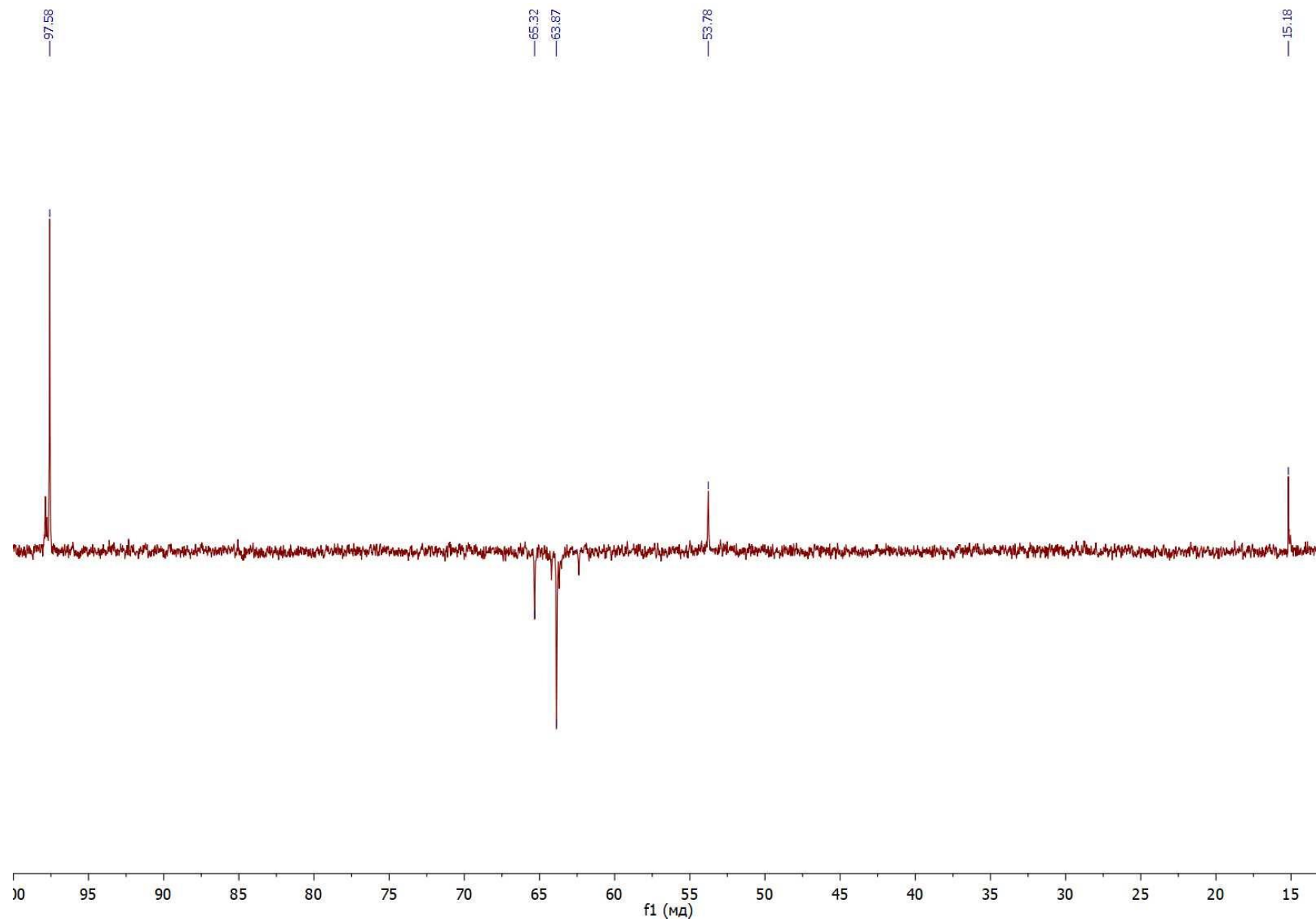


Figure S15. ^{13}C (dept) NMR spectrum of compound **1e** (101 MHz, CDCl_3)

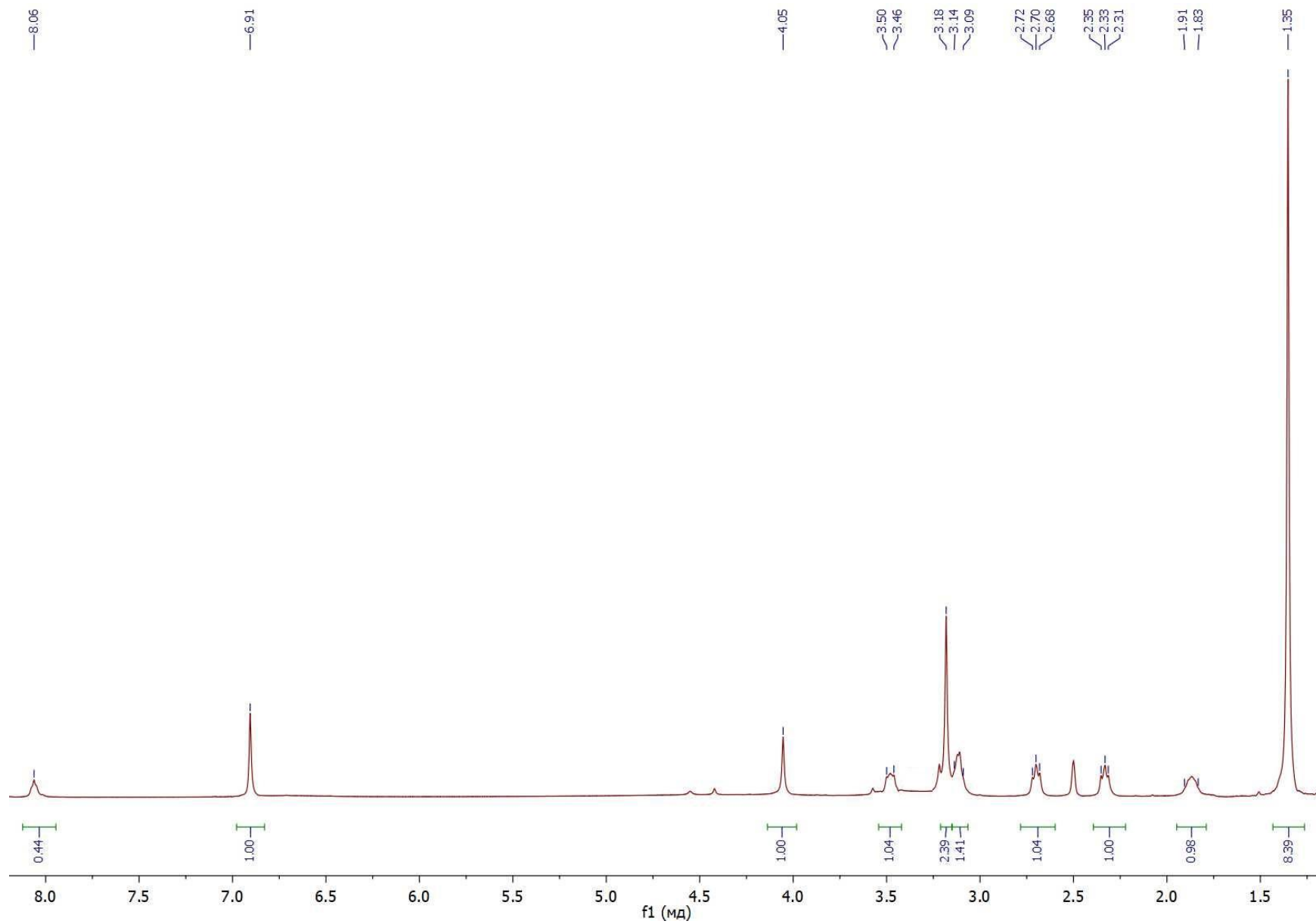


Figure S16. ^1H NMR spectrum of compound **1f** (400 MHz, $\text{DMSO-}d_6$)

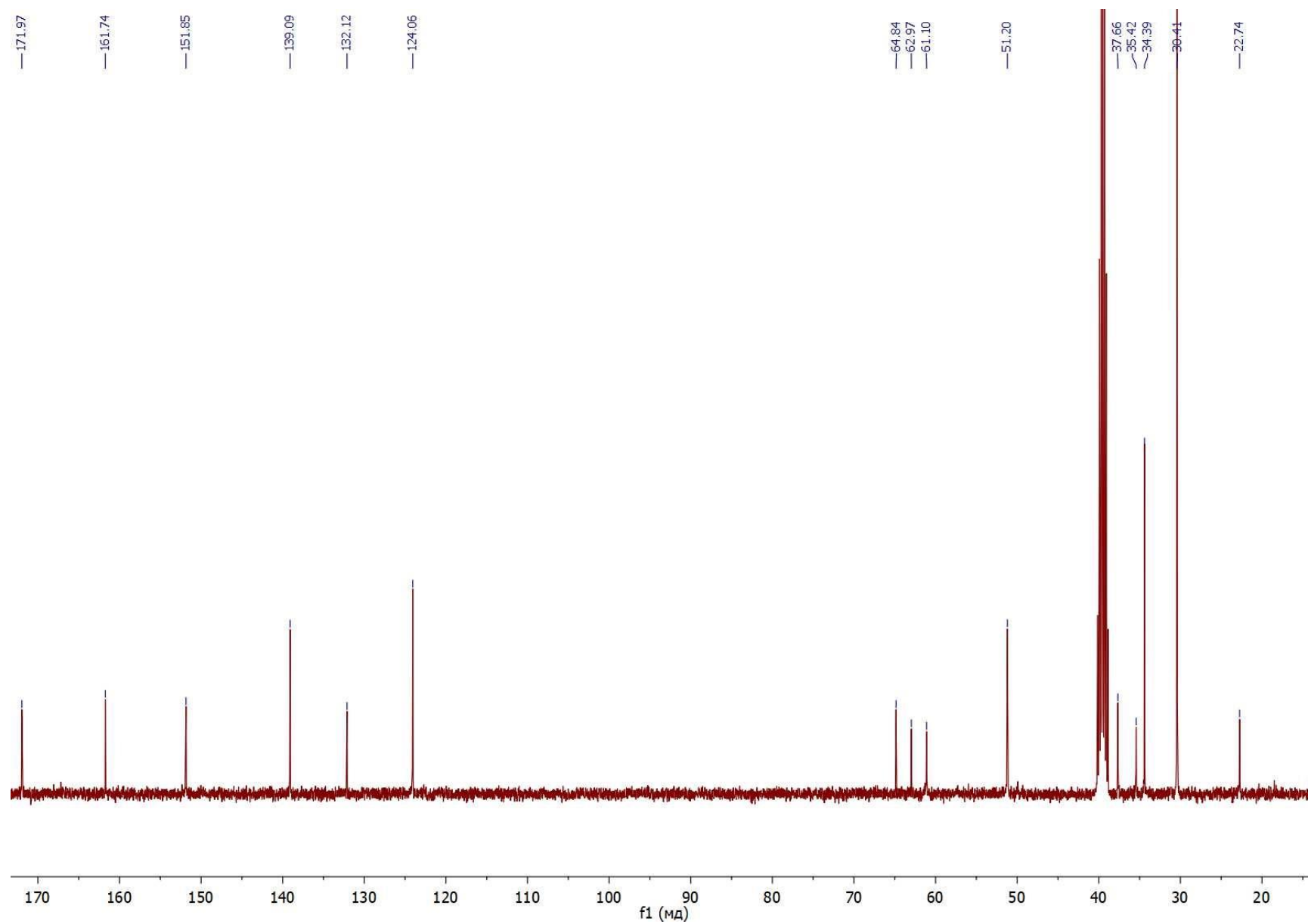


Figure S17. ^{13}C - $\{^1\text{H}\}$ NMR spectrum of compound **1f** (101 MHz, $\text{DMSO}-d_6$)

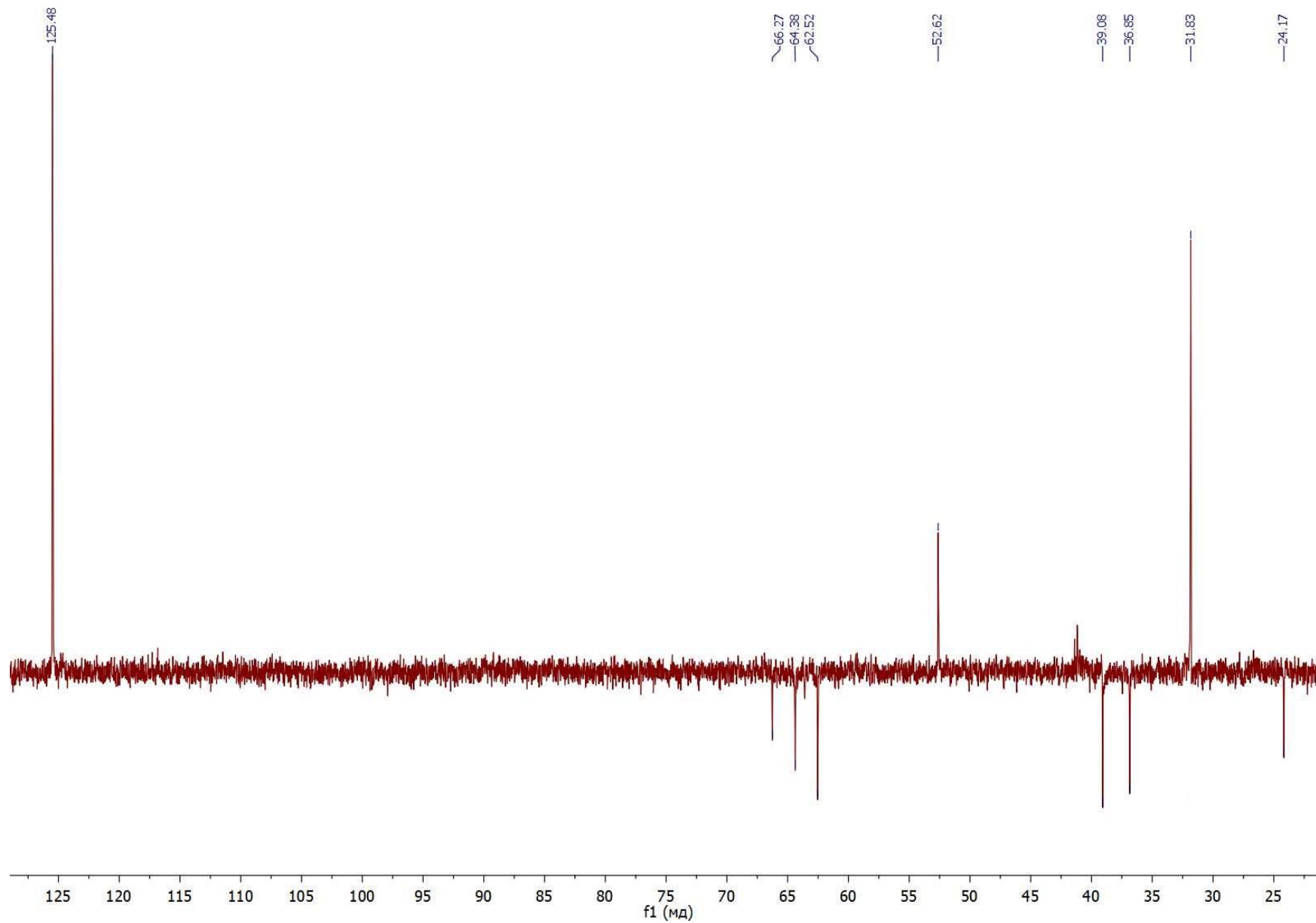


Figure S18. ¹³C (dept) NMR spectrum of compound **1f** (101 MHz, DMSO-*d*₆)

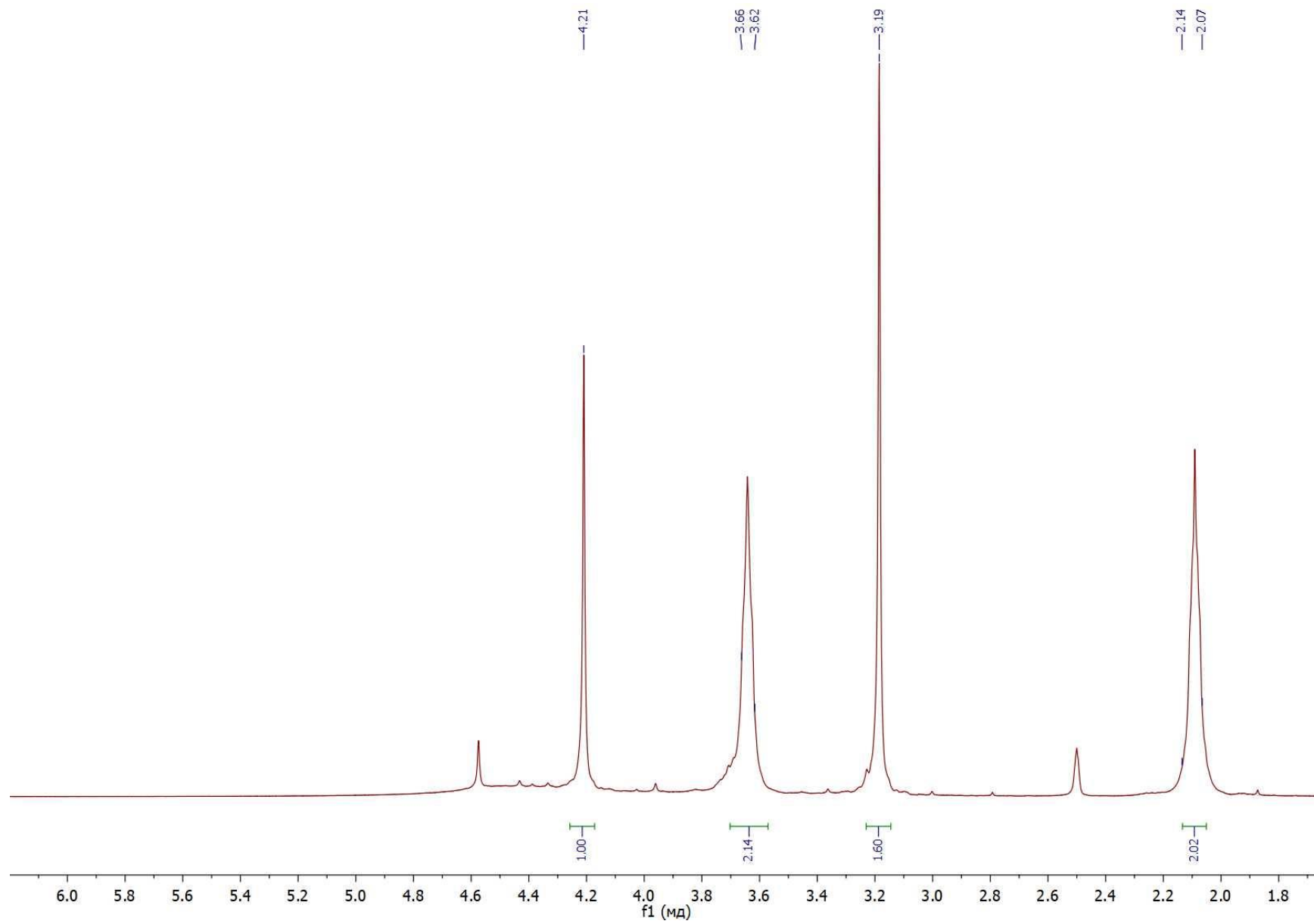


Figure S19. ^1H NMR spectrum of compound **1g** (400 MHz, $\text{DMSO}-d_6$)

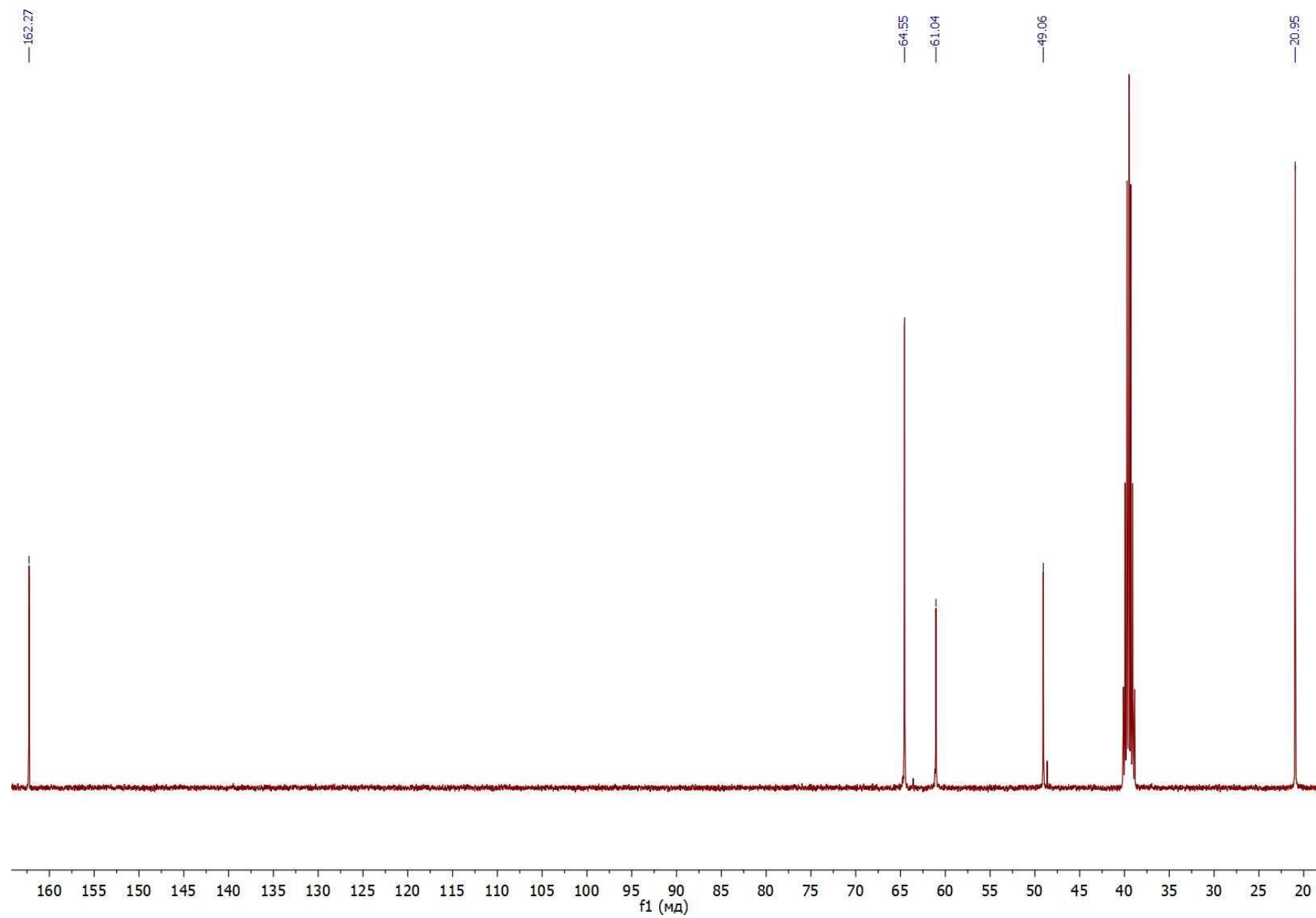


Figure S20. ^{13}C - $\{^1\text{H}\}$ NMR spectrum of compound **1g** (101 MHz, $\text{DMSO-}d_6$)

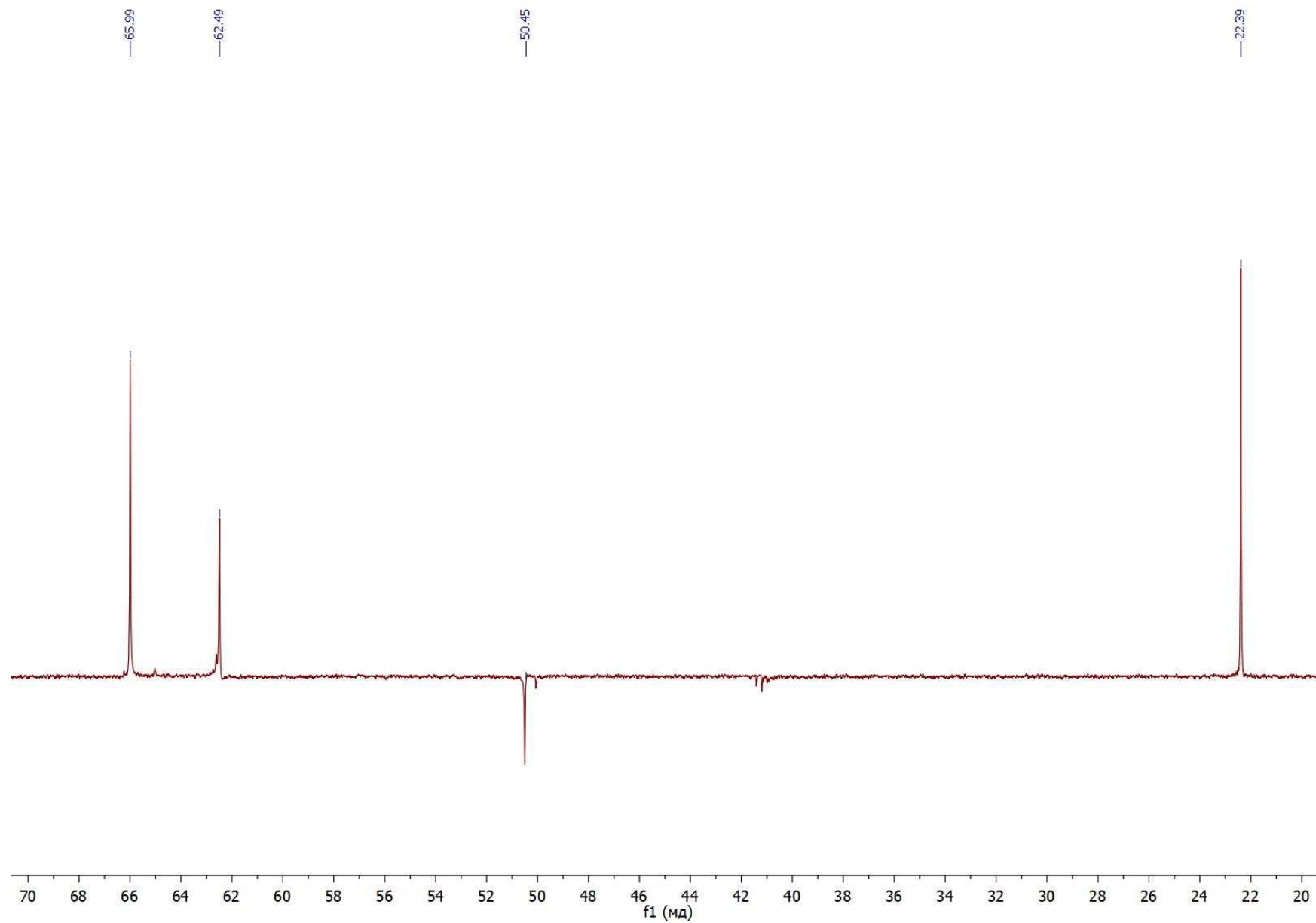


Figure S21. ^{13}C (dept) NMR spectrum of compound **1g** (101 MHz, $\text{DMSO}-d_6$)

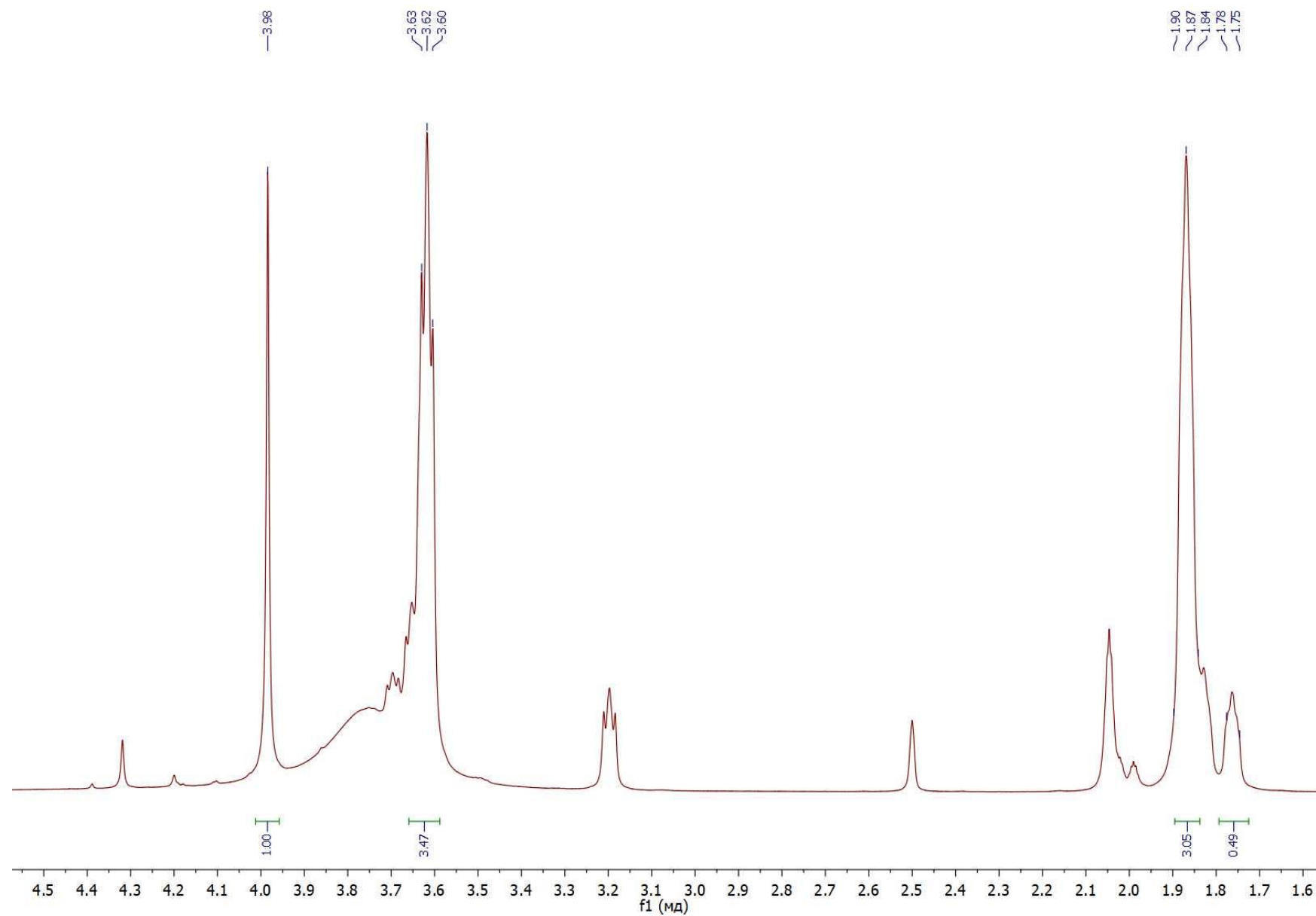


Figure S22. ¹H NMR spectrum of compound **1h** (600 MHz, DMSO-*d*₆)

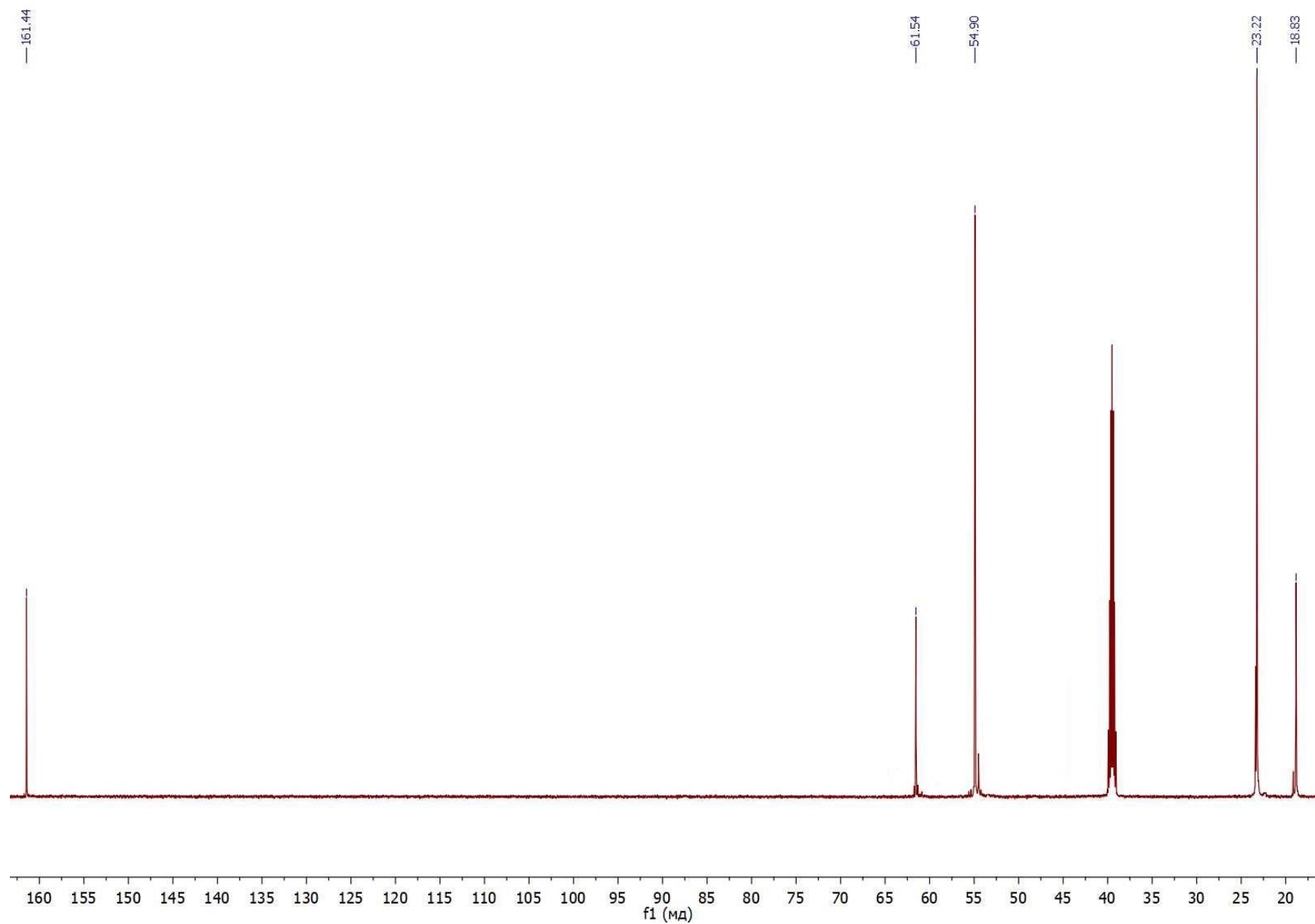


Figure S23. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **1h** (101 MHz, $\text{DMSO-}d_6$)

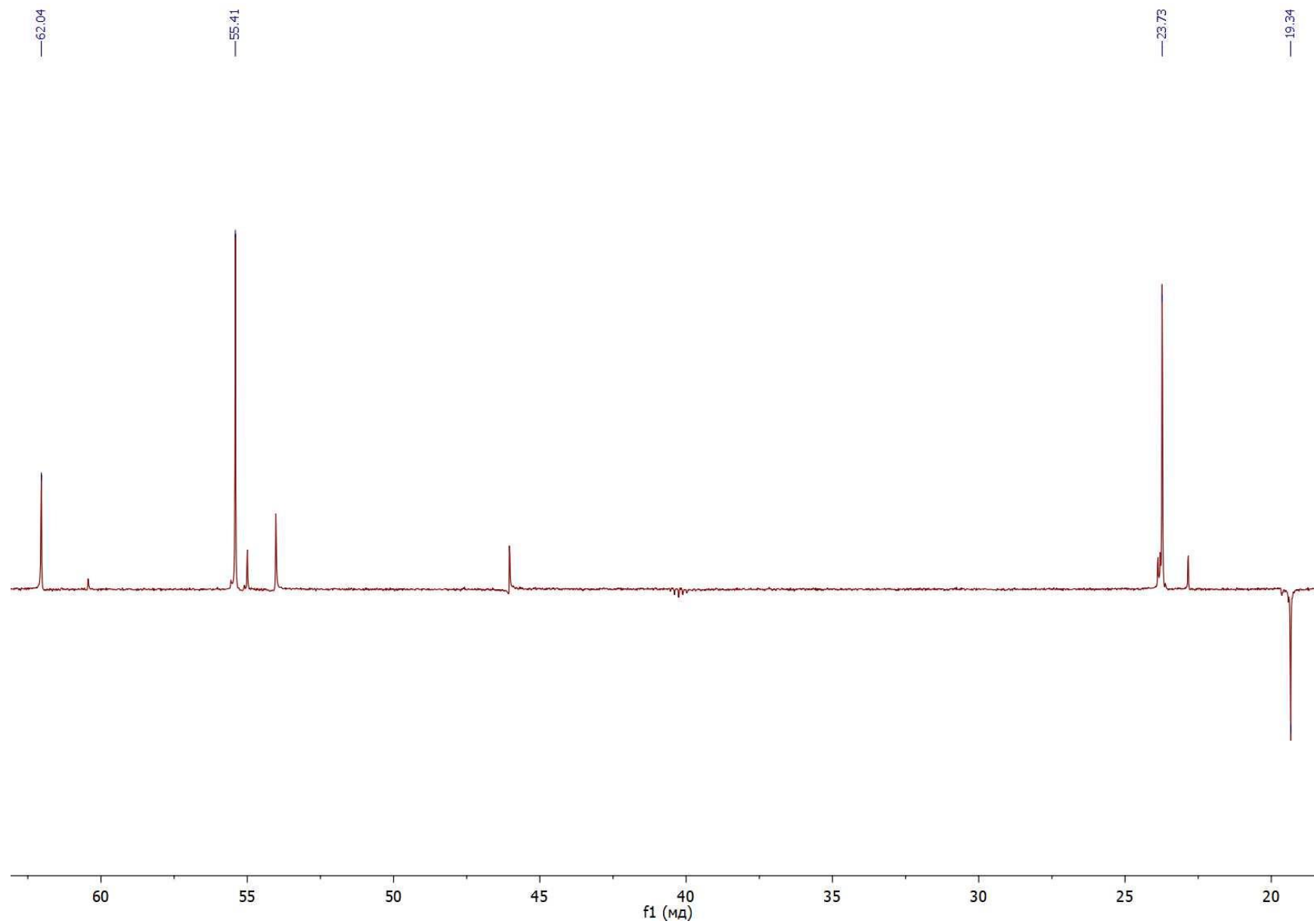


Figure S24. ^{13}C (dept) NMR spectrum of compound **1h** (101 MHz, $\text{DMSO}-d_6$)

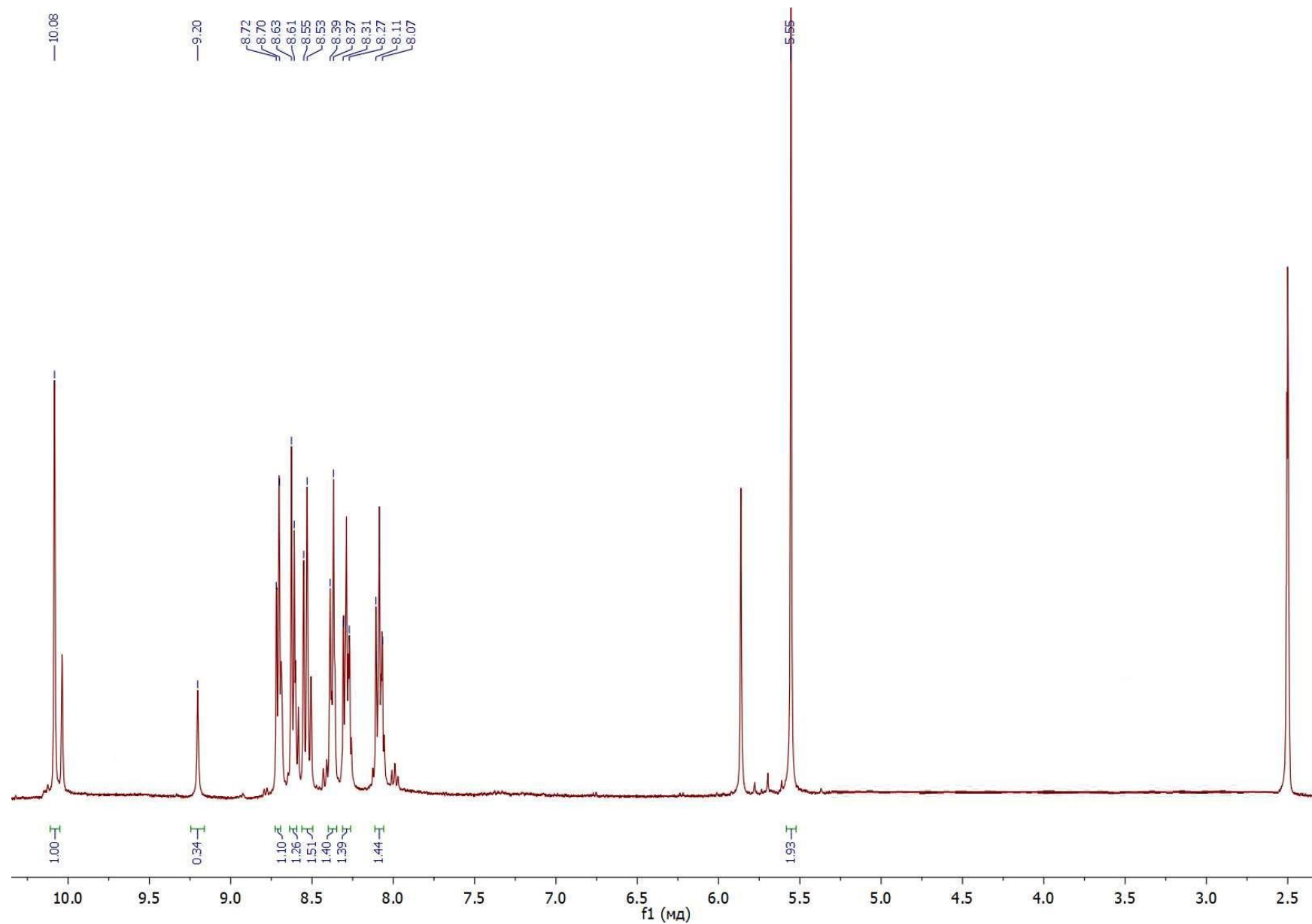


Figure S25. ¹H NMR spectrum of compound **1i** (400 MHz, DMSO-*d*₆)

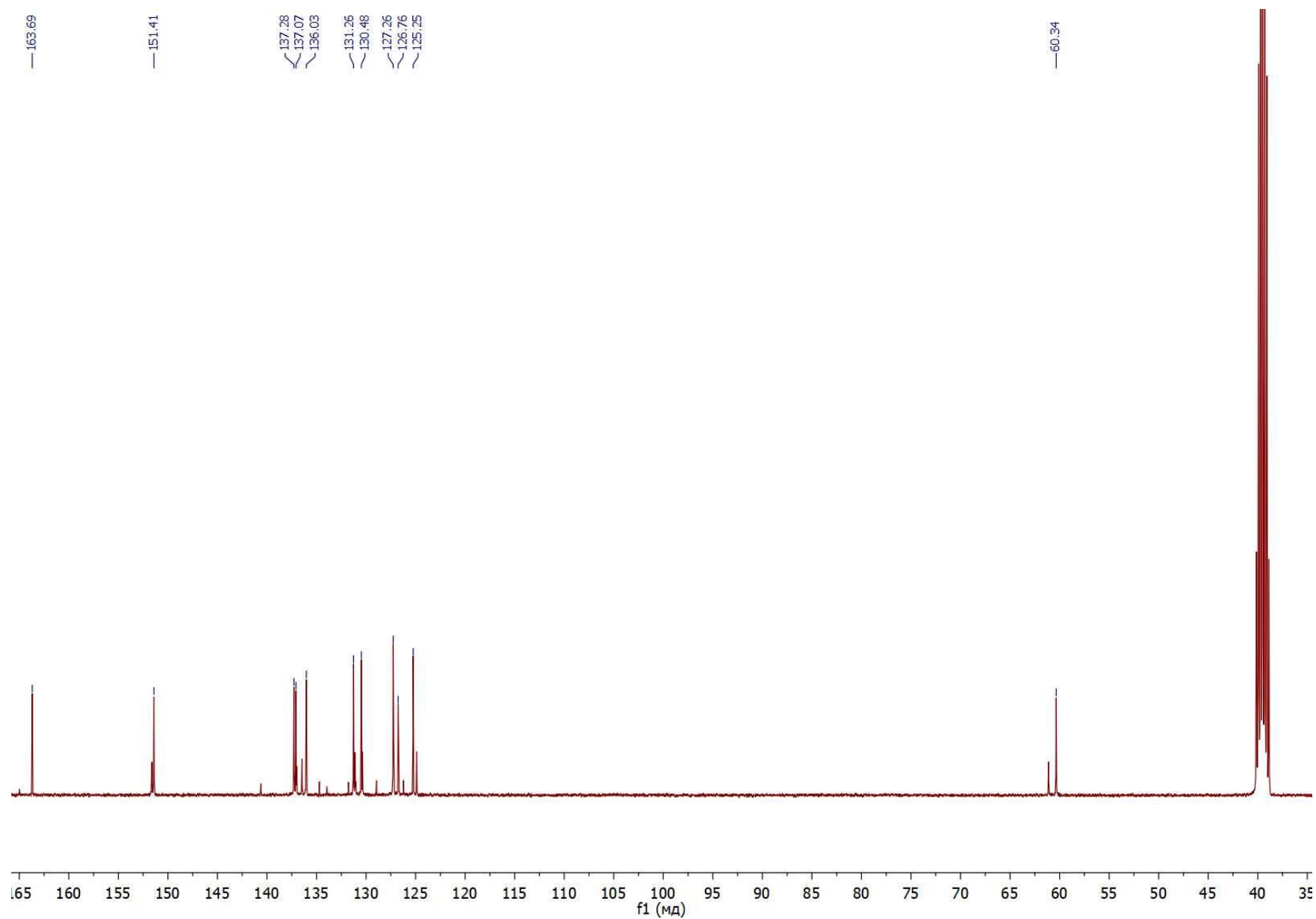


Figure S26. ^{13}C - $\{^1\text{H}\}$ NMR spectrum of compound **1i** (101 MHz, DMSO- d_6)

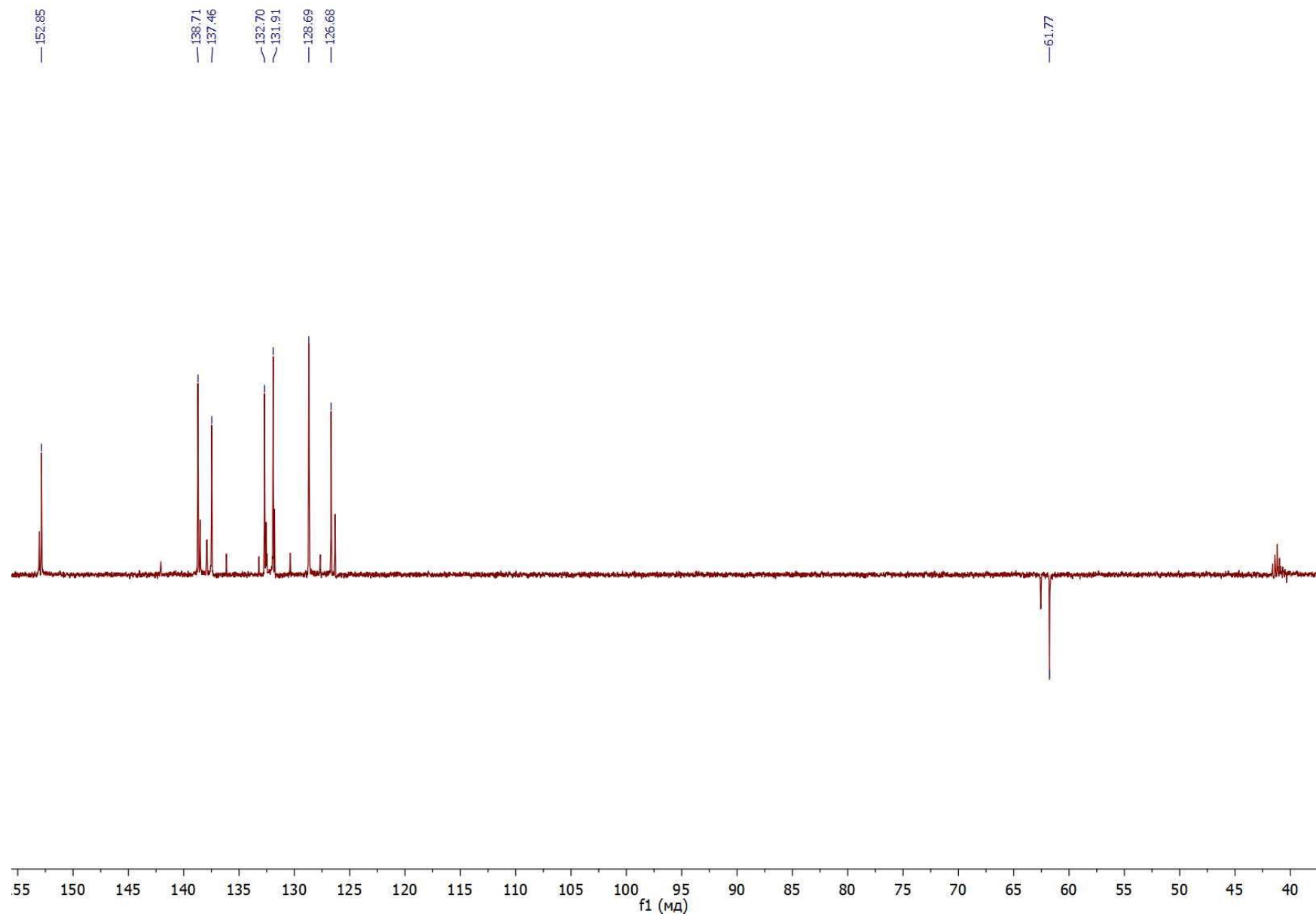


Figure S27. ^{13}C (dept) NMR spectrum of compound **1i** (101 MHz, $\text{DMSO}-d_6$)

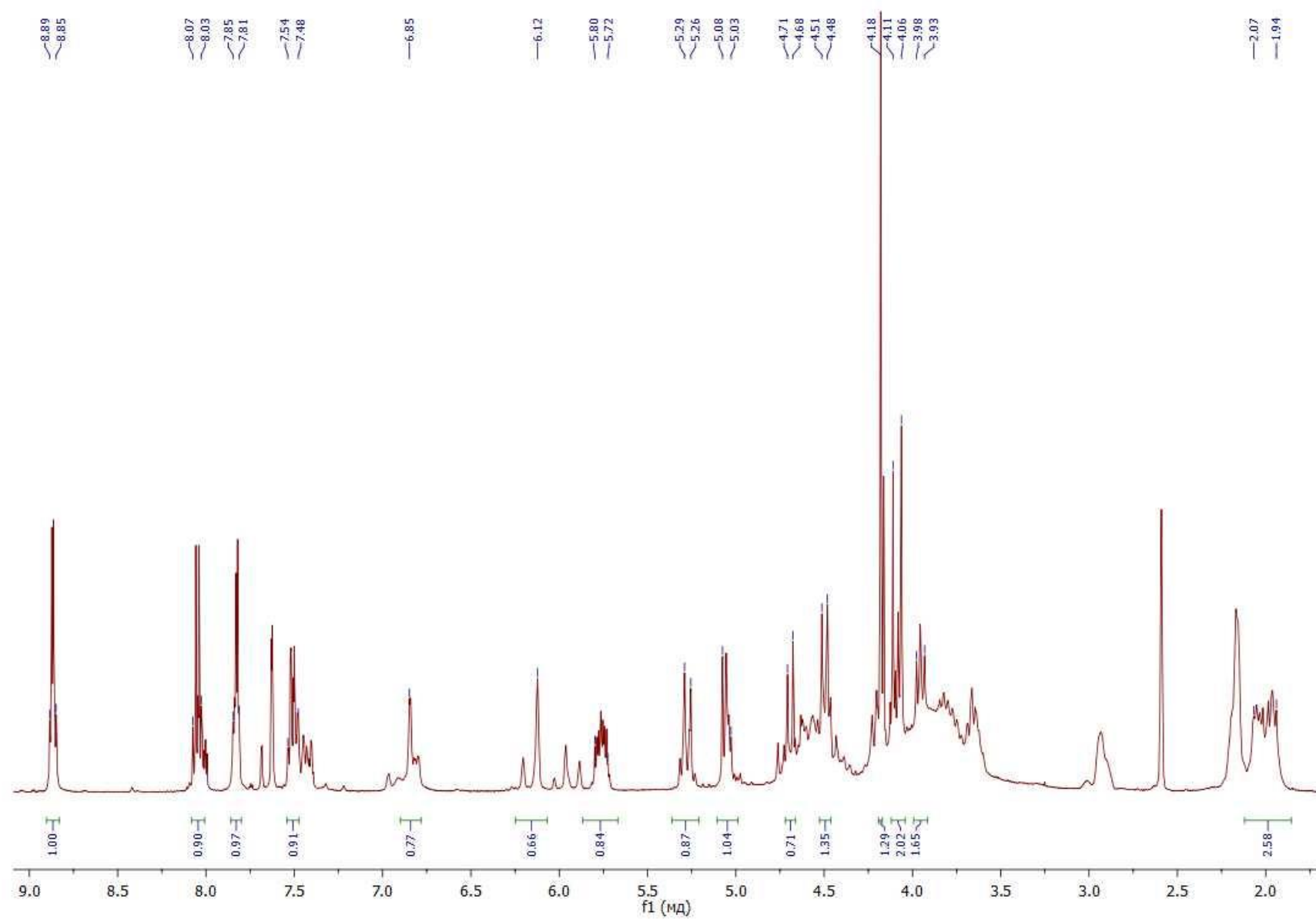


Figure S28. ¹H NMR spectrum of compound **1j** (500 MHz, DMSO-*d*₆)

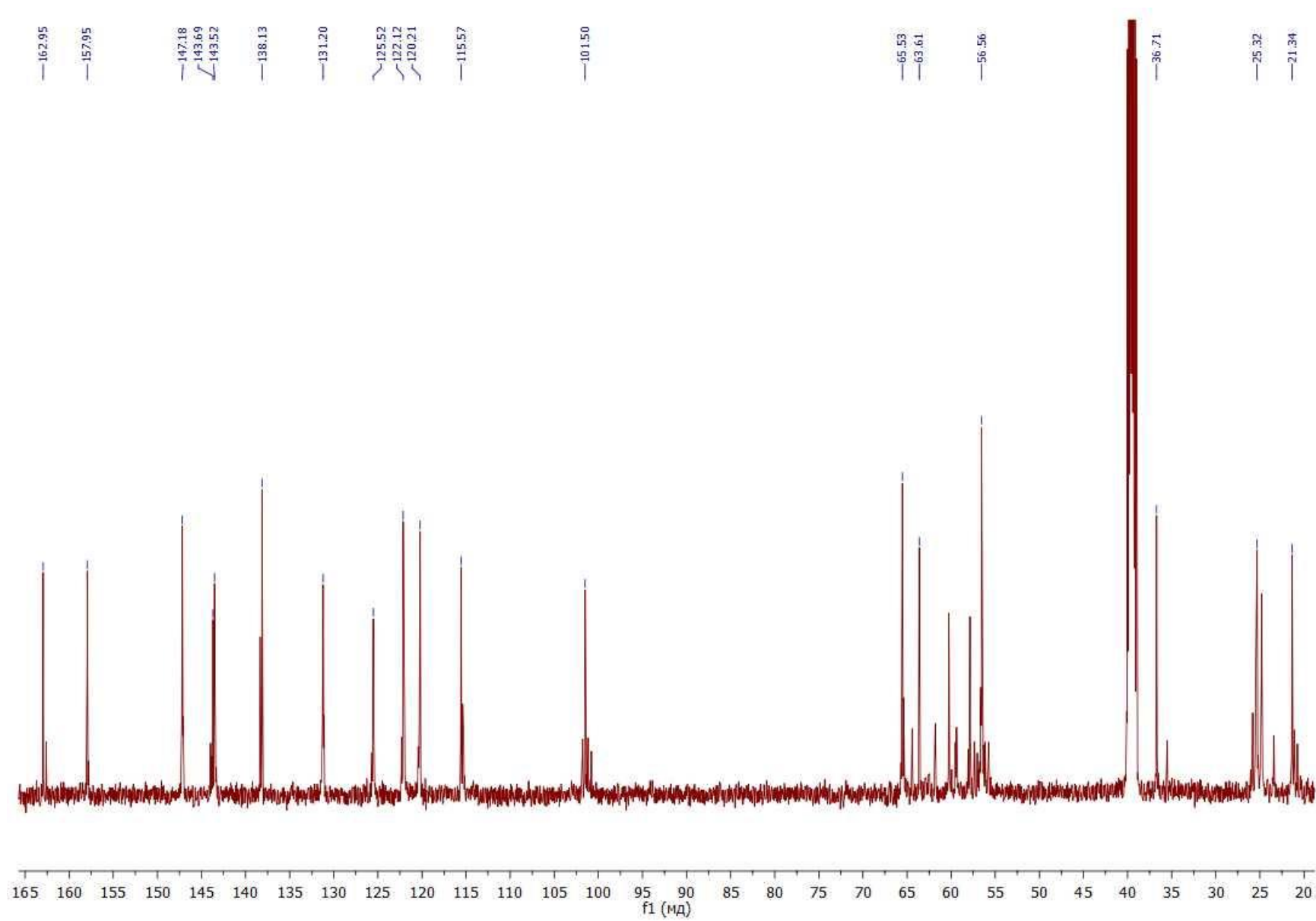


Figure S29. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **1j** (126 MHz, $\text{DMSO}-d_6$)

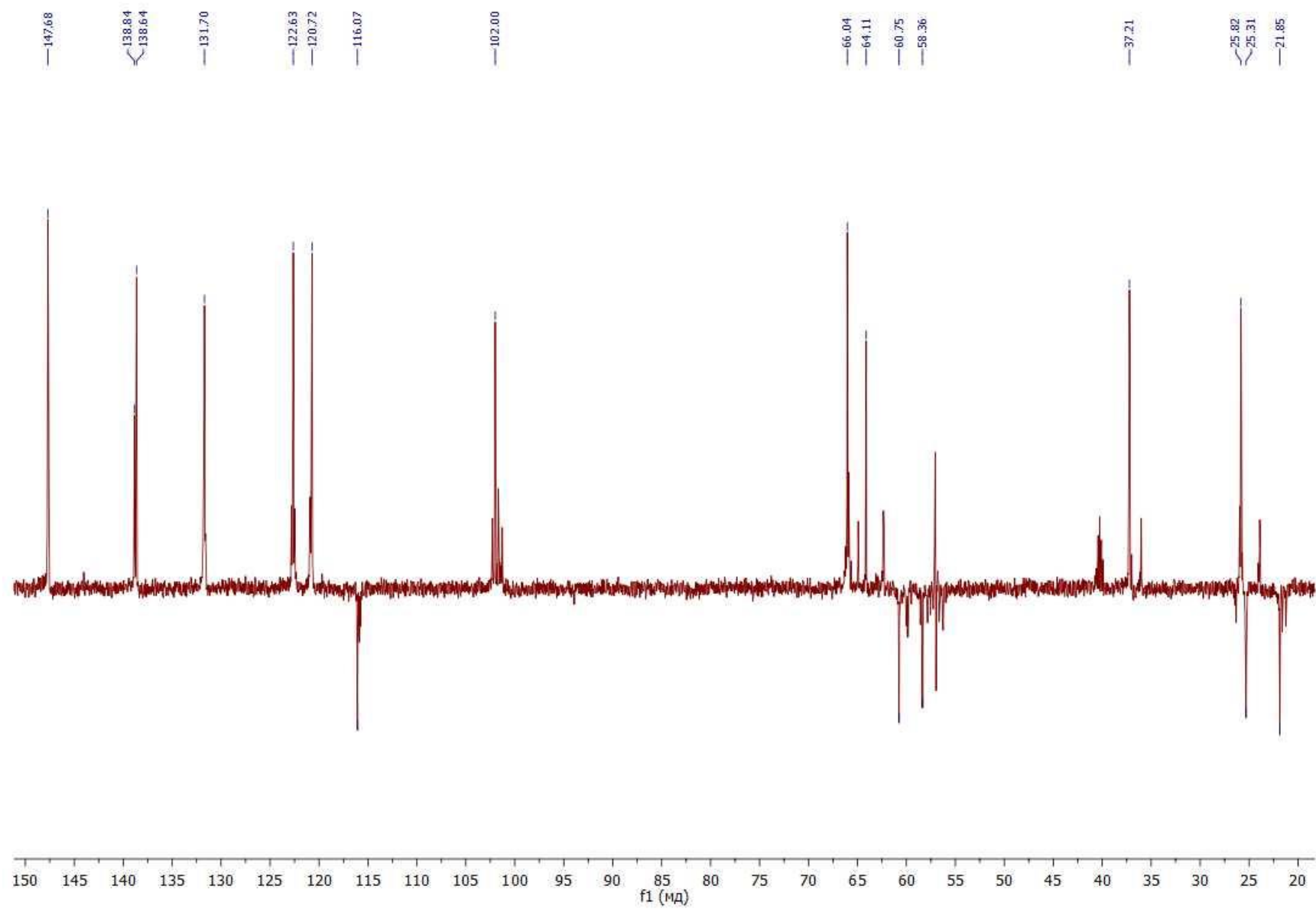


Figure S30. ^{13}C (dept) NMR spectrum of compound **1j** (126 MHz, $\text{DMSO-}d_6$)

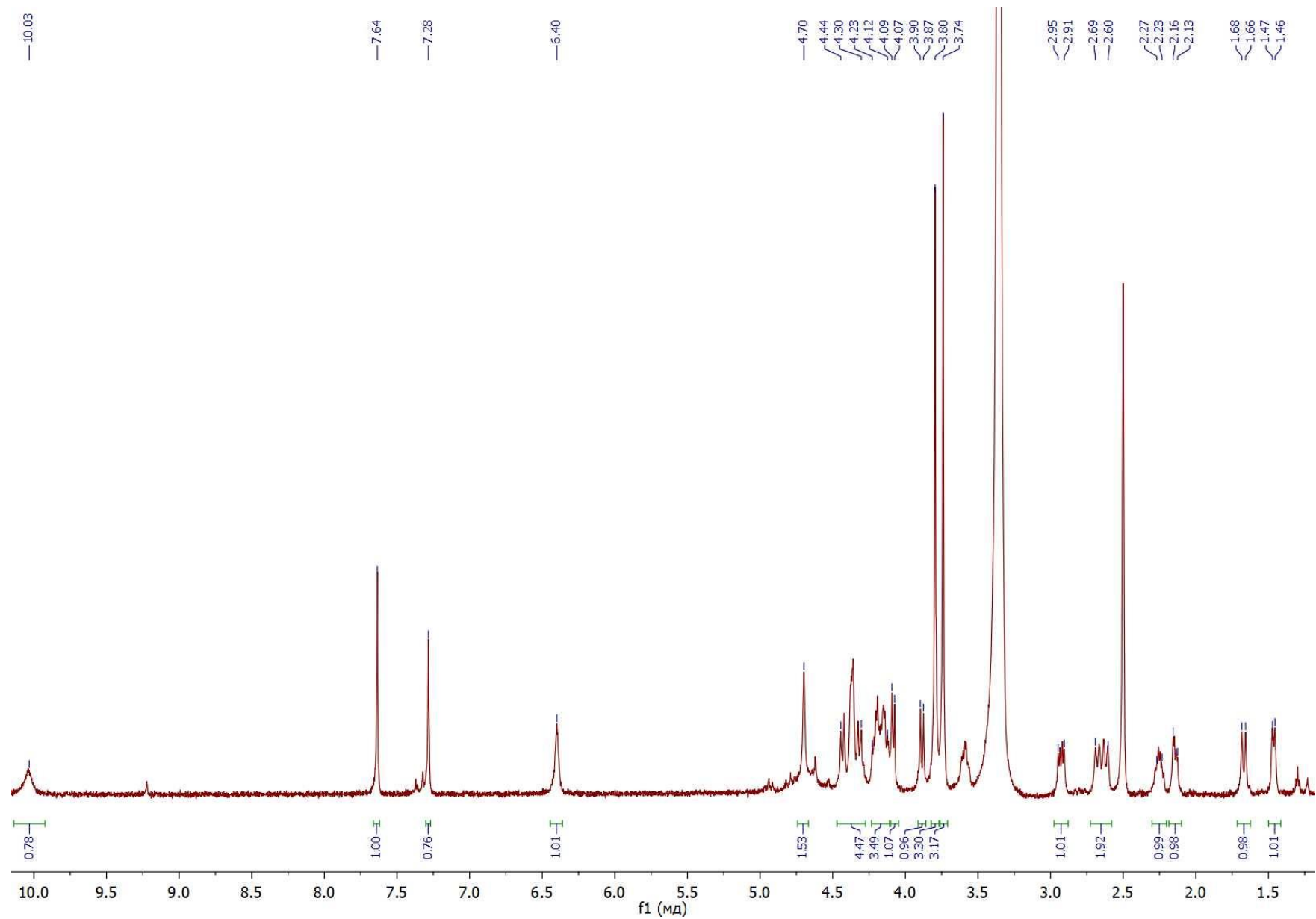


Figure S31. ¹H NMR spectrum of compound **1k** (400 MHz, DMSO-*d*₆)

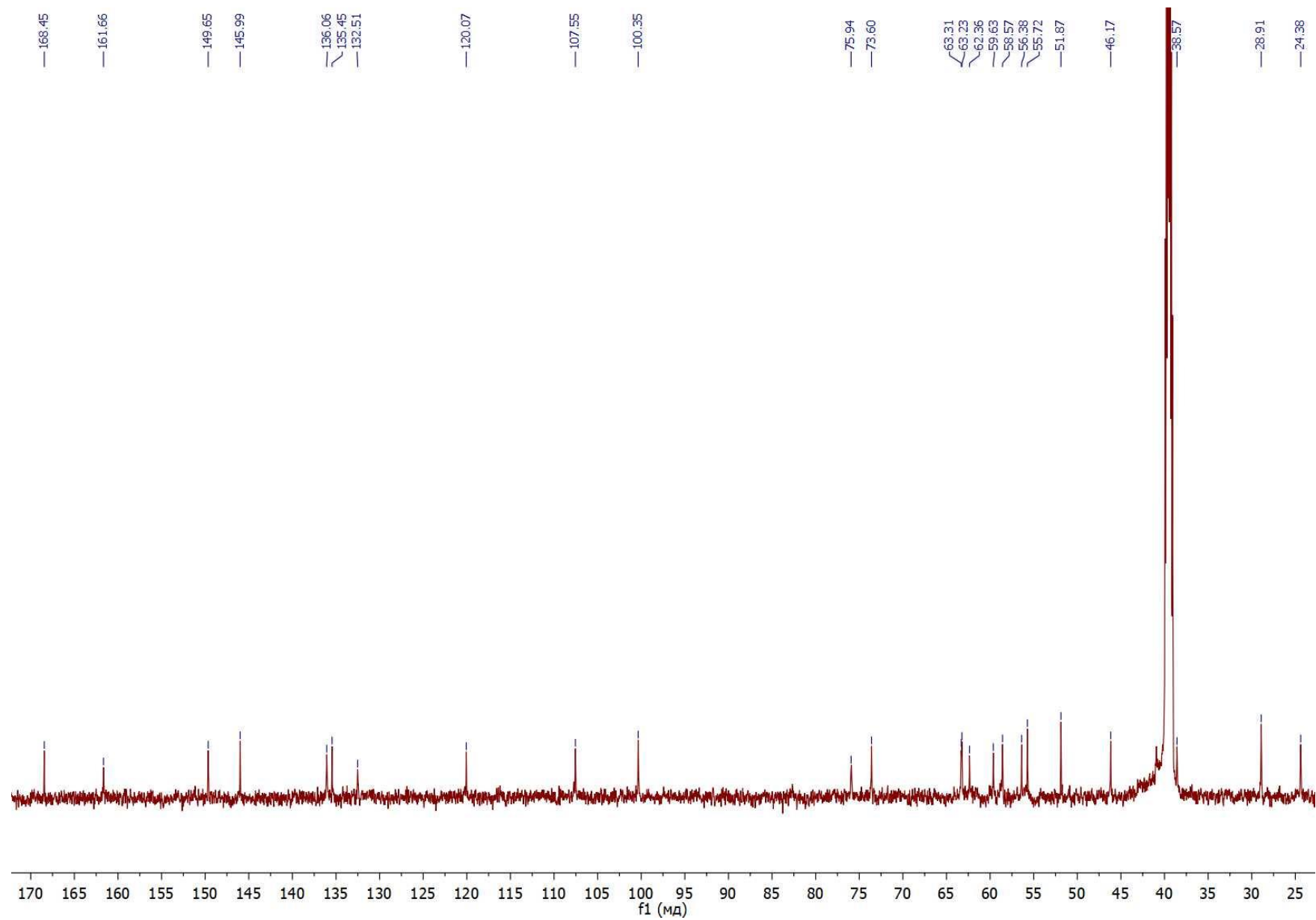


Figure S32. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **1k** (101 MHz, $\text{DMSO}-d_6$)

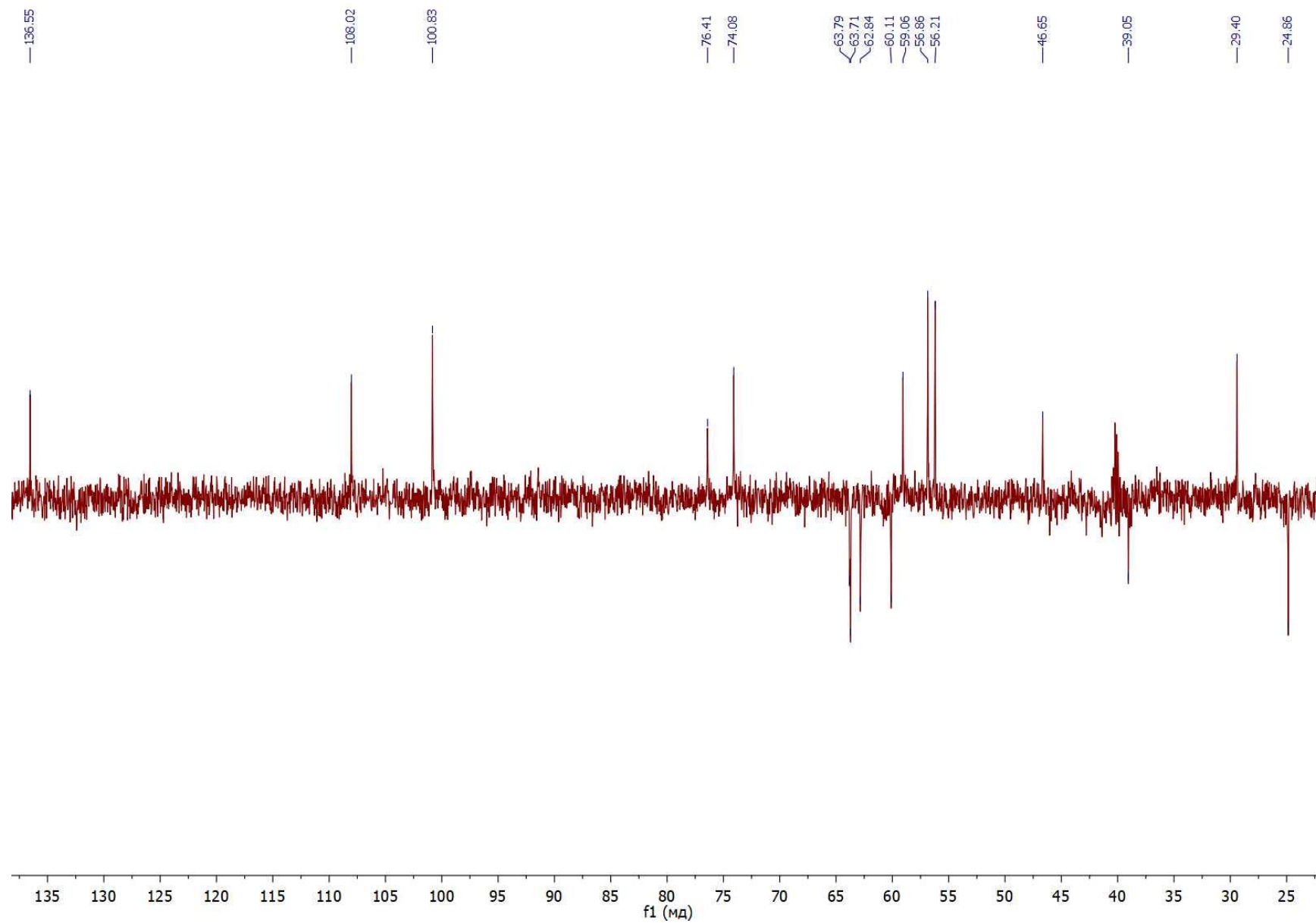


Figure S33. ^{13}C (dept) NMR spectrum of compound **1k** (101 MHz, $\text{DMSO-}d_6$)

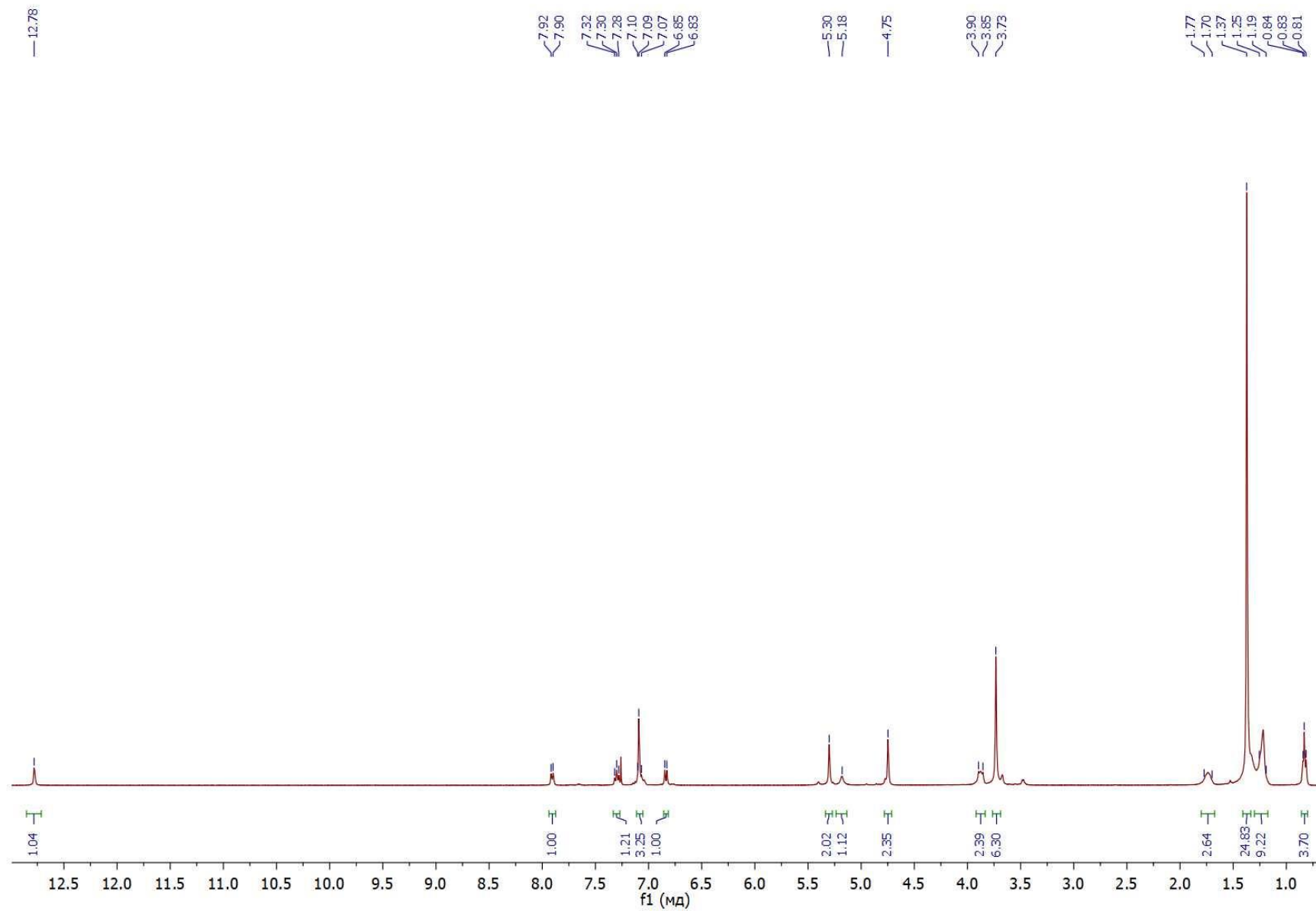


Figure S34. ¹H NMR spectrum of compound **3a** (600 MHz, CDCl₃)

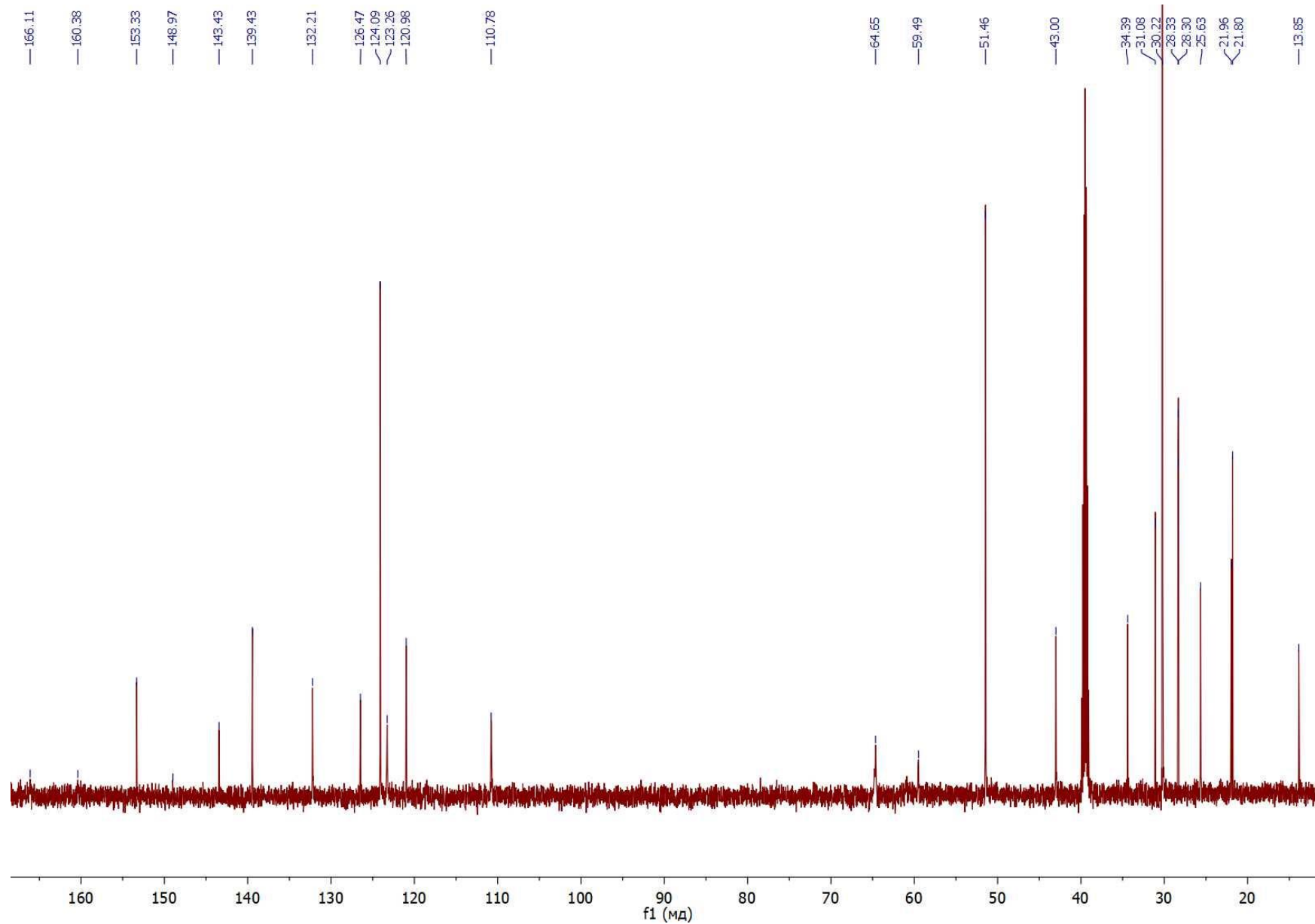


Figure S35. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **3a** (151 MHz, $\text{DMSO}-d_6$)

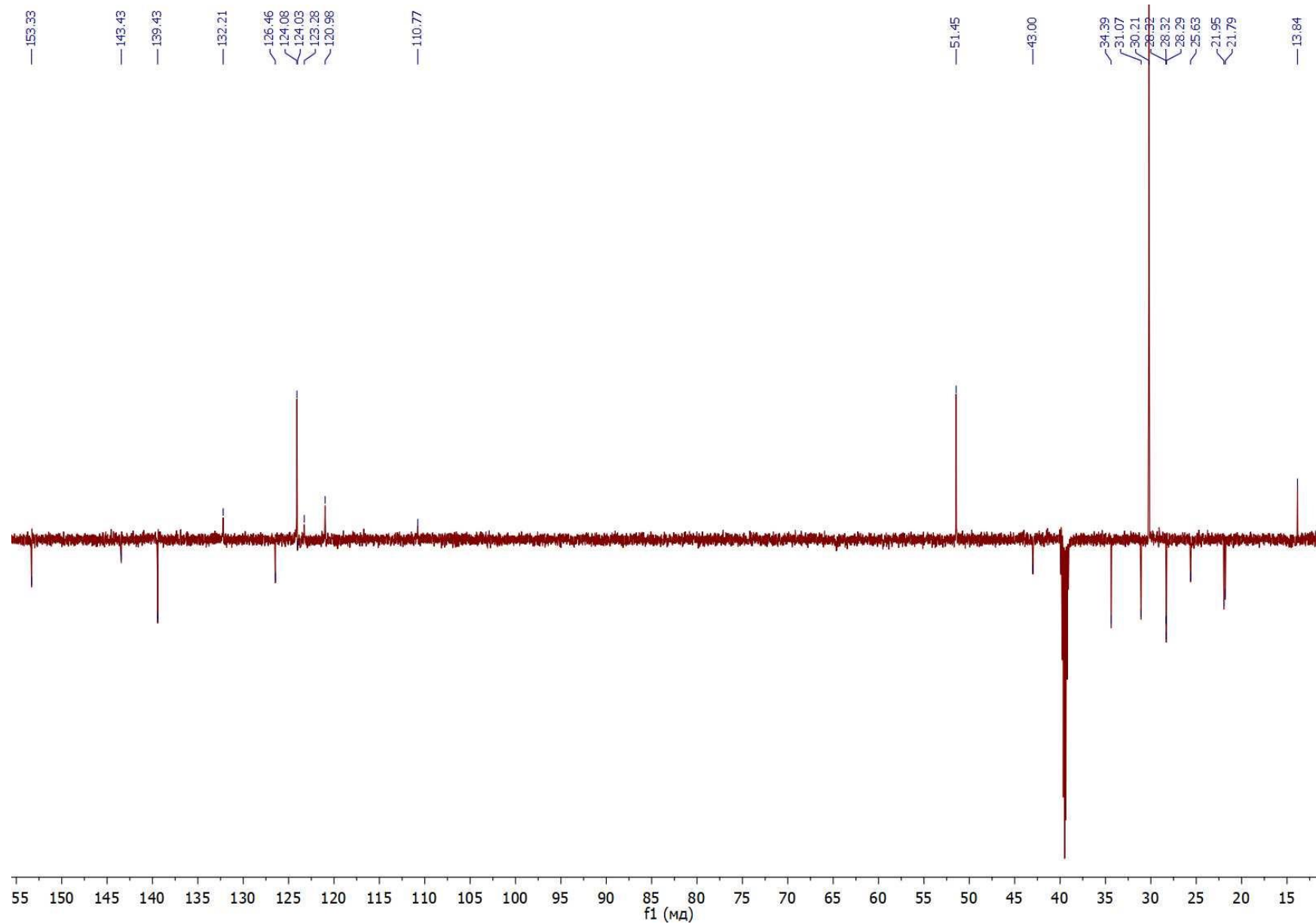


Figure S36. ¹³C (JMOD) NMR spectrum of compound **3a** (151 MHz, DMSO-*d*₆)

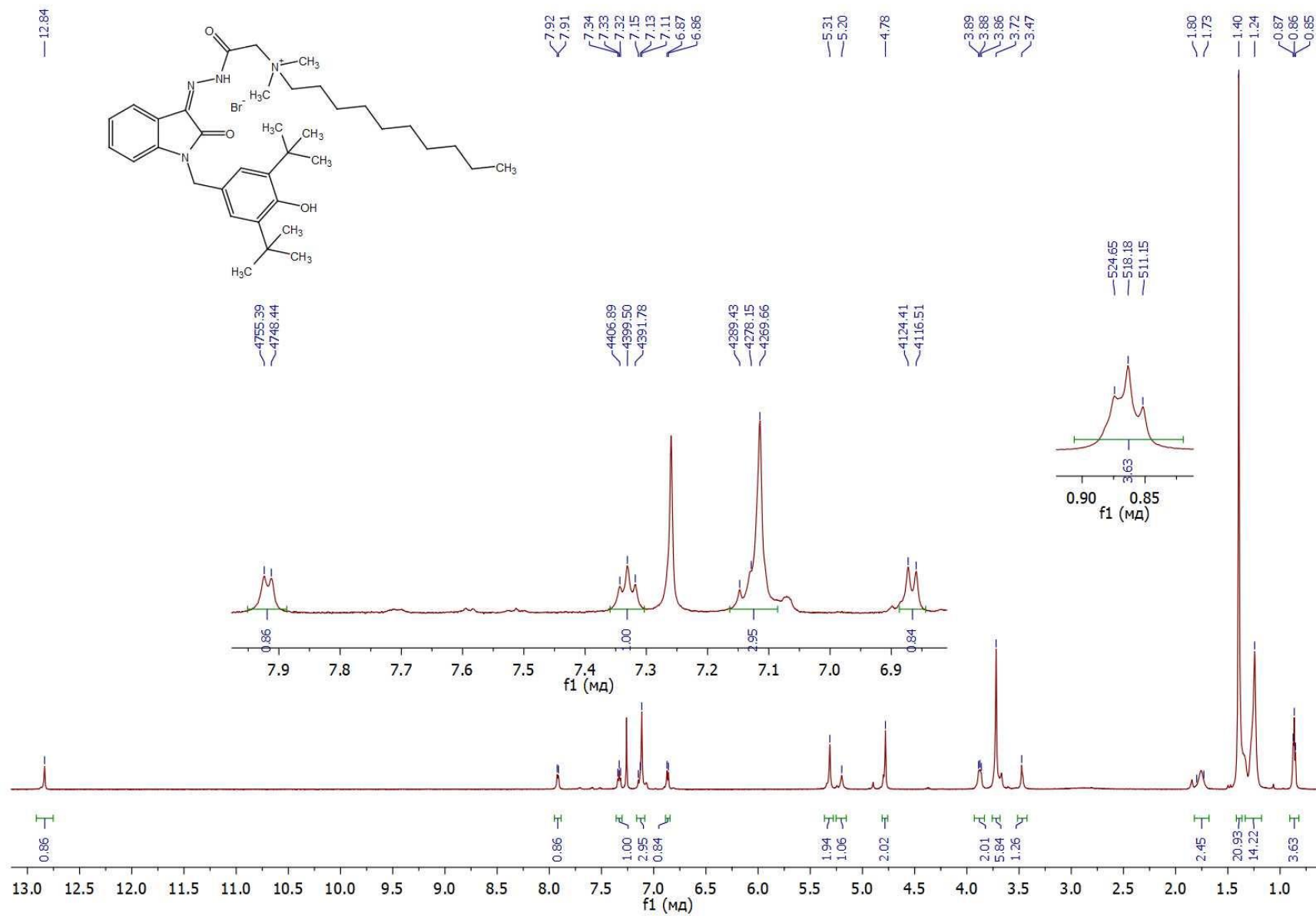


Figure S37. ¹H NMR spectrum of compound **3b** (600 MHz, CDCl₃)

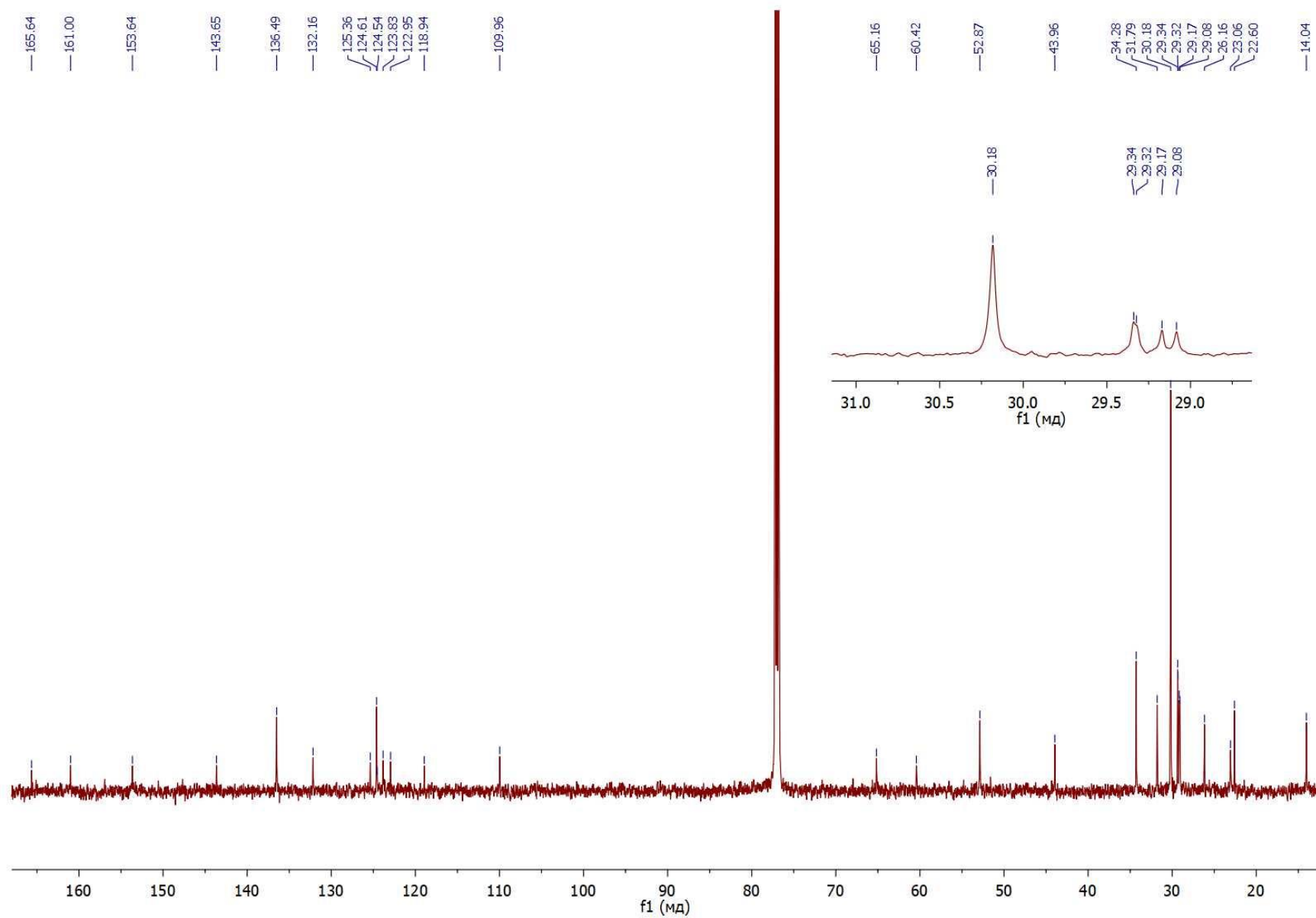


Figure S38. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **3b** (151 MHz, CDCl_3)

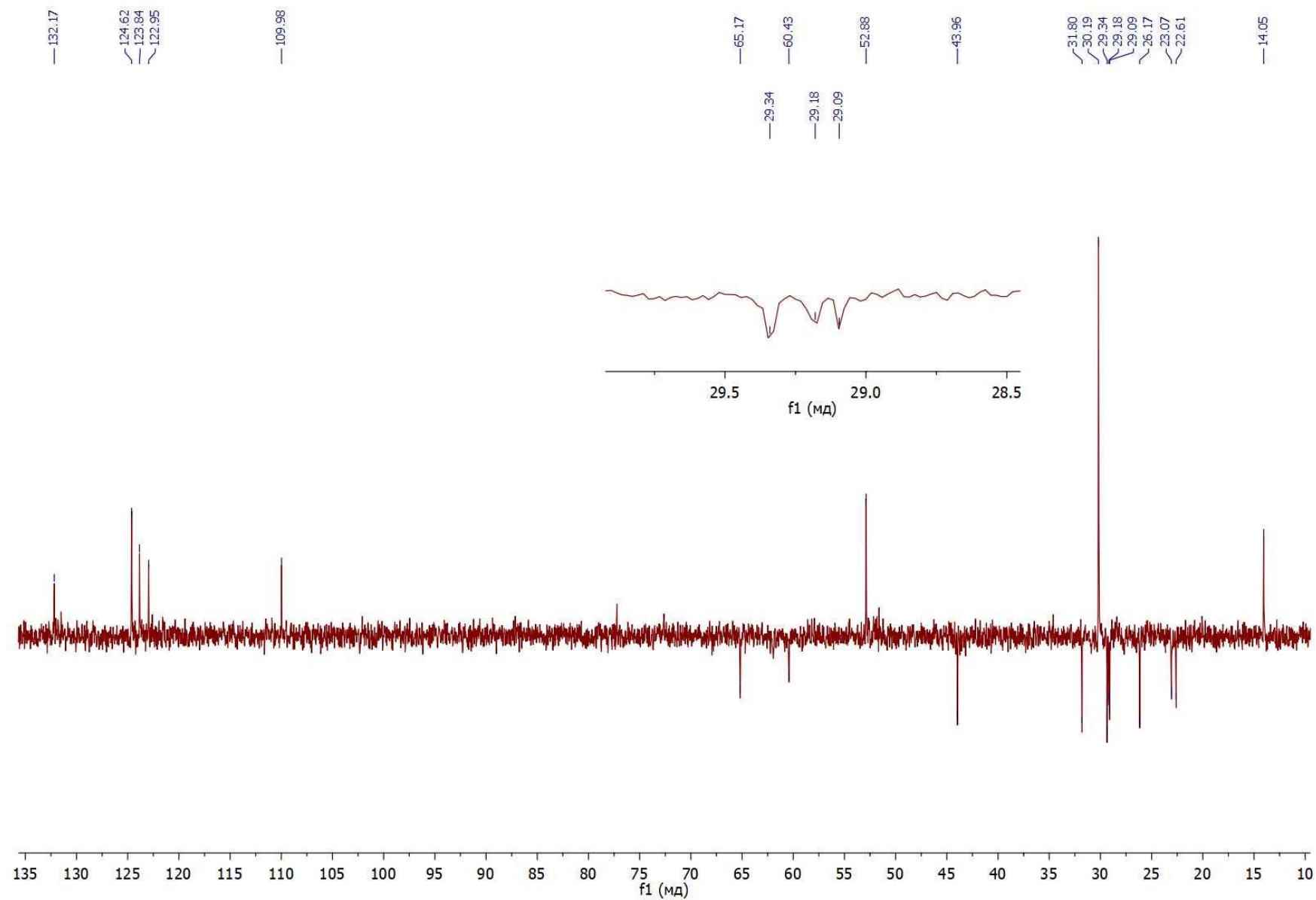


Figure S39. ^{13}C (dept) NMR spectrum of compound **3b** (151 MHz, CDCl_3)

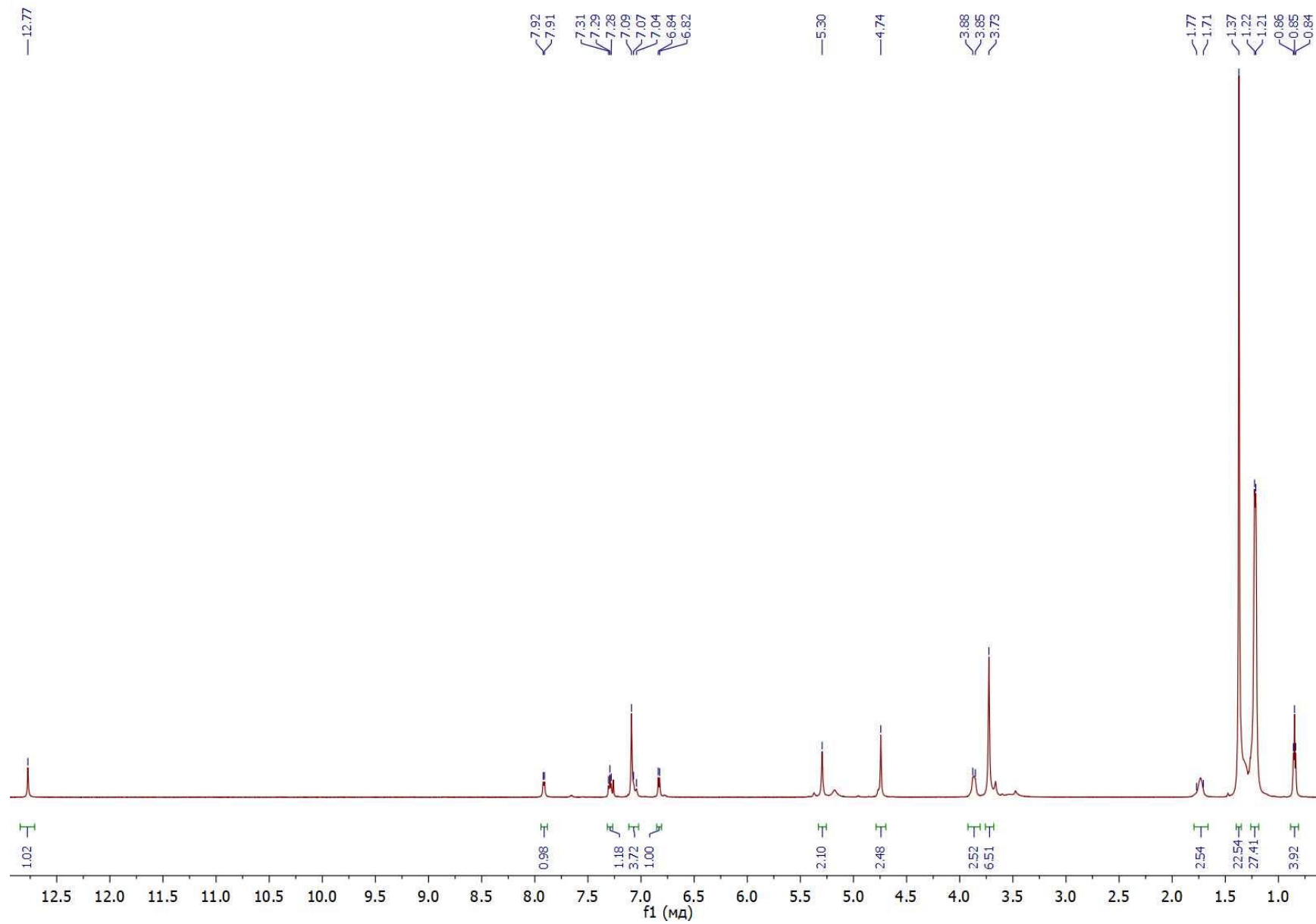


Figure S40. ¹H NMR spectrum of compound **3c** (400 MHz, CDCl₃)

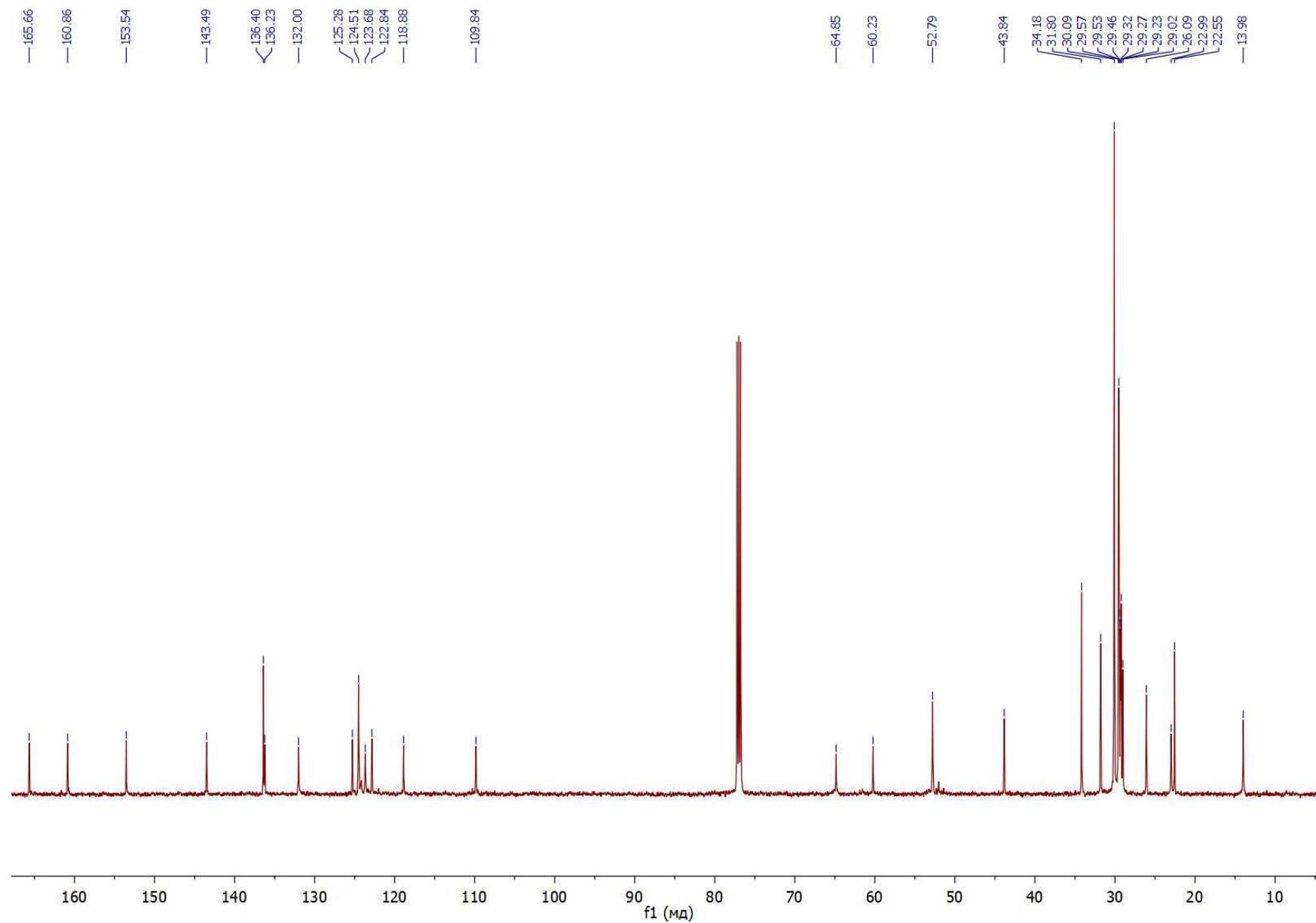


Figure S41. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **3c** (101 MHz, CDCl_3)

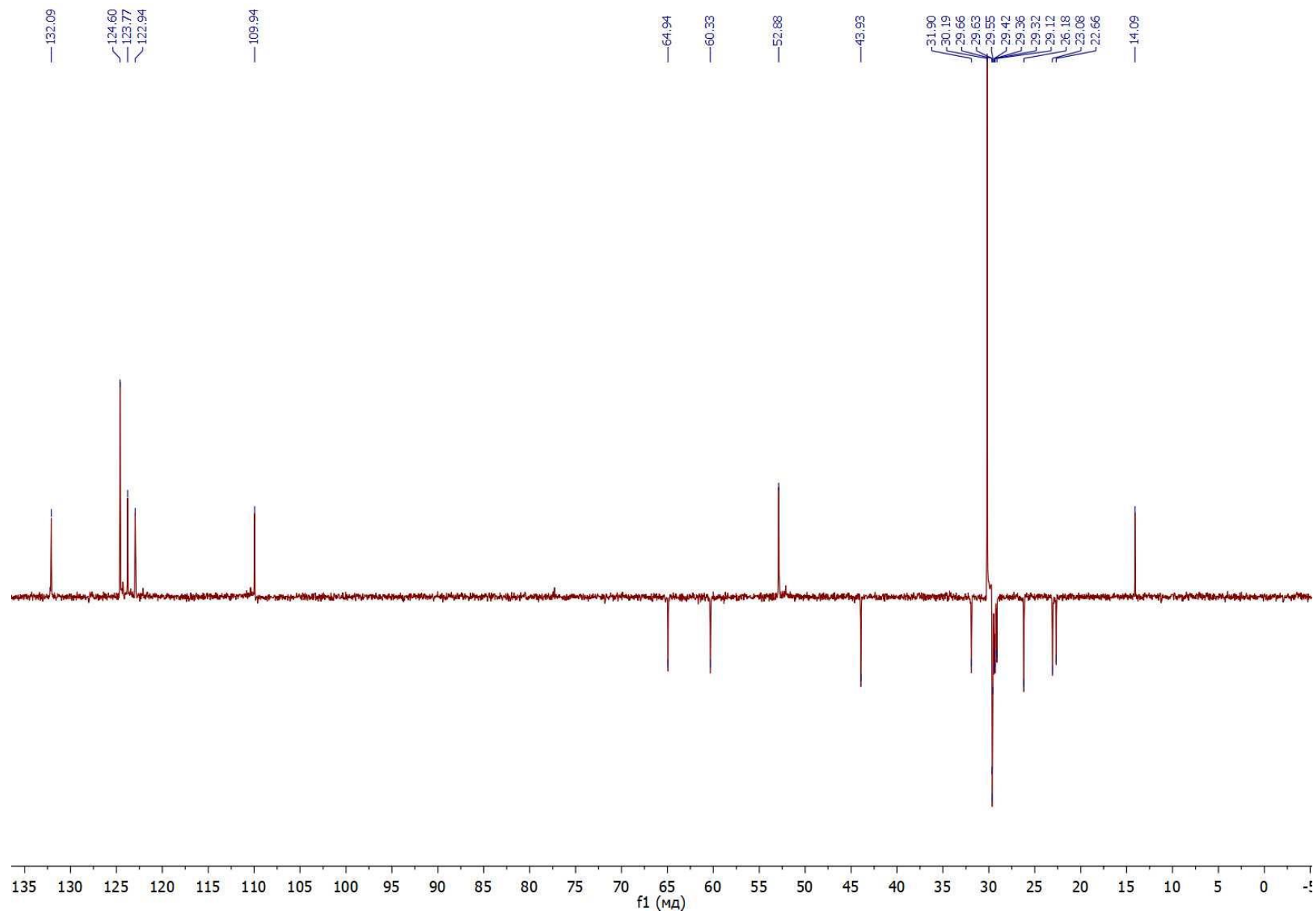


Figure S42. ^{13}C (dept) NMR spectrum of compound **3c** (101 MHz, CDCl_3)

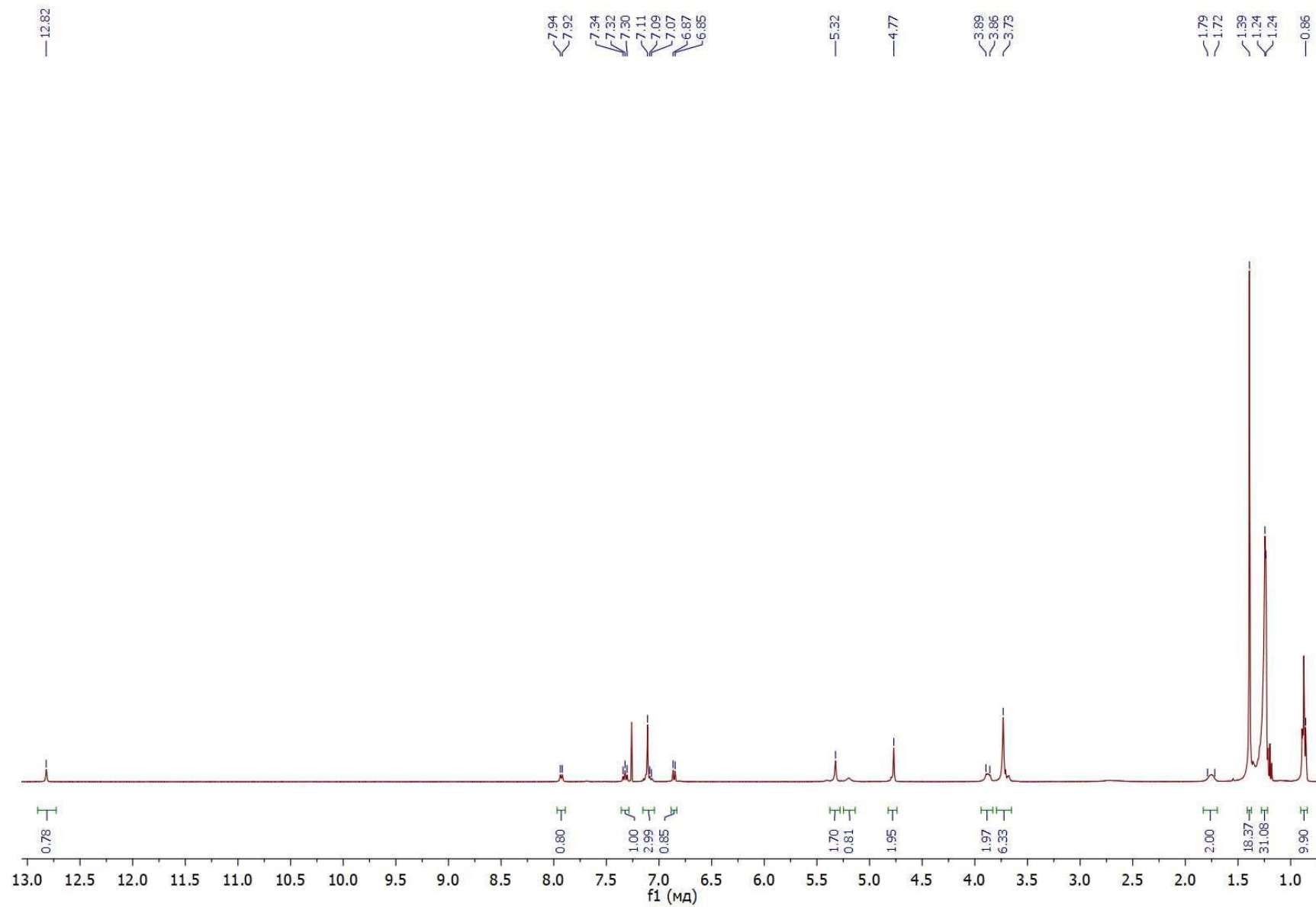


Figure S43. ¹H NMR spectrum of compound **3d** (400 MHz, CDCl₃)

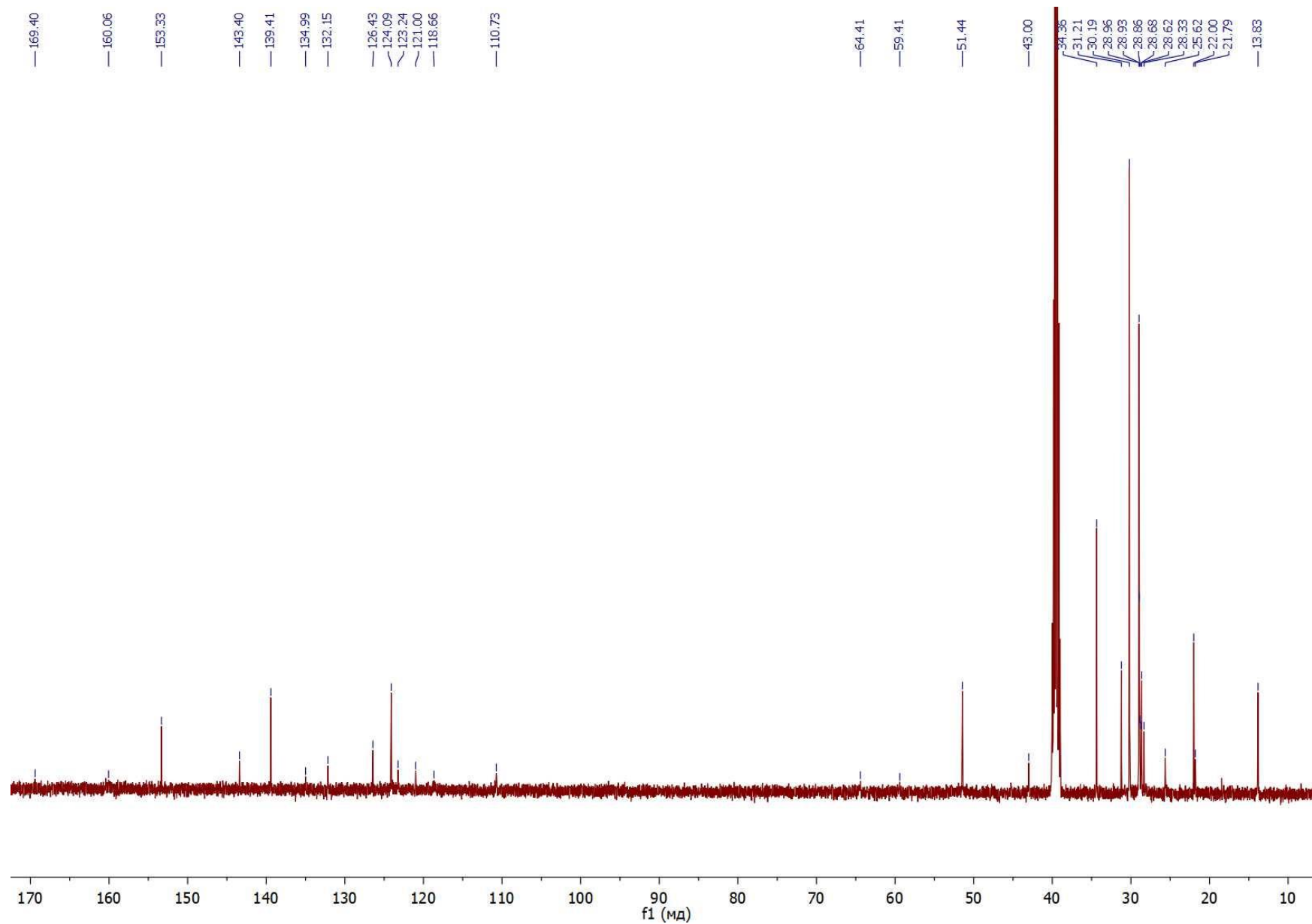


Figure S44. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **3d** (101 MHz, $\text{DMSO}-d_6$)

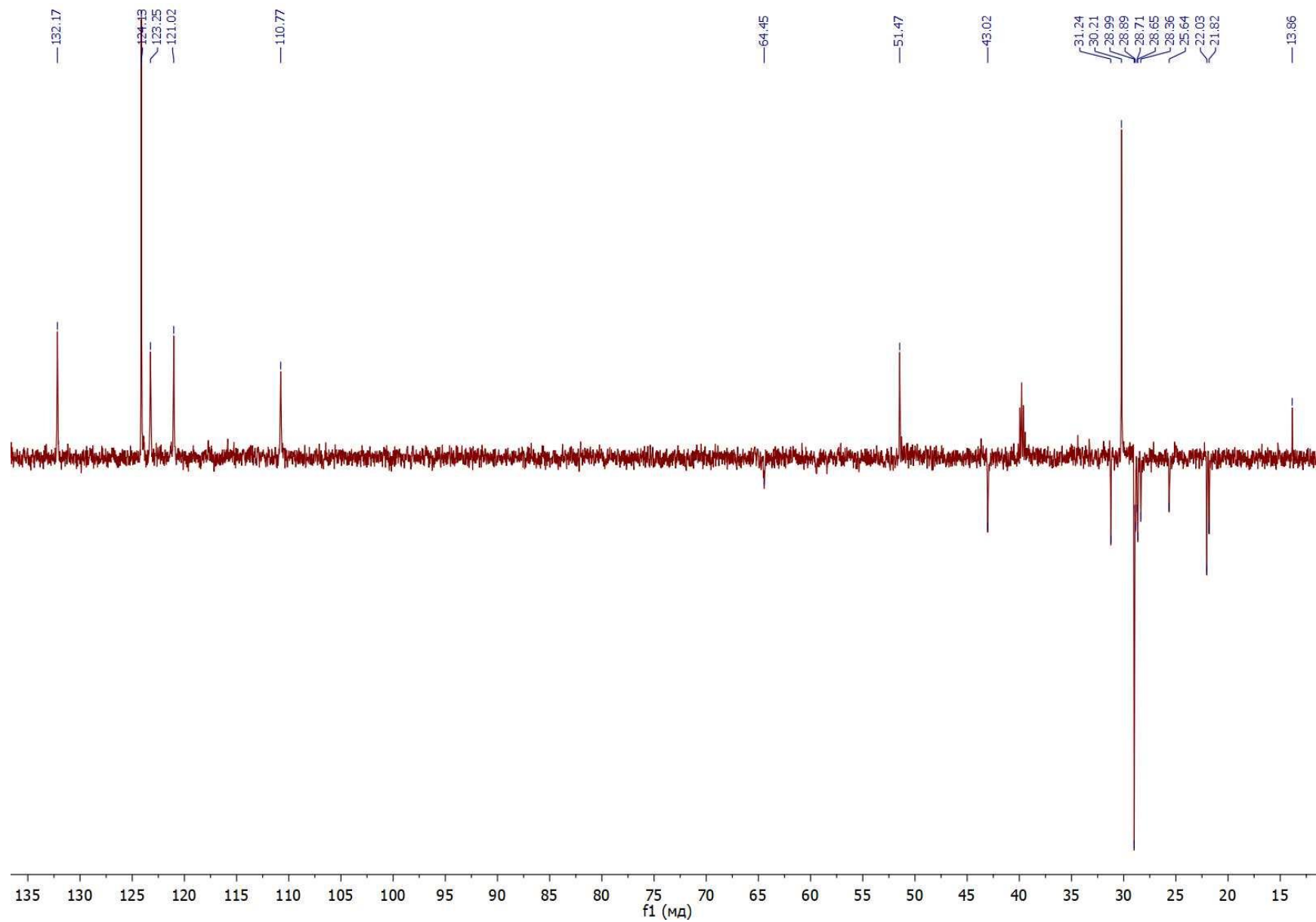


Figure S45. ^{13}C (dept) NMR spectrum of compound **3d** (101 MHz, $\text{DMSO-}d_6$)

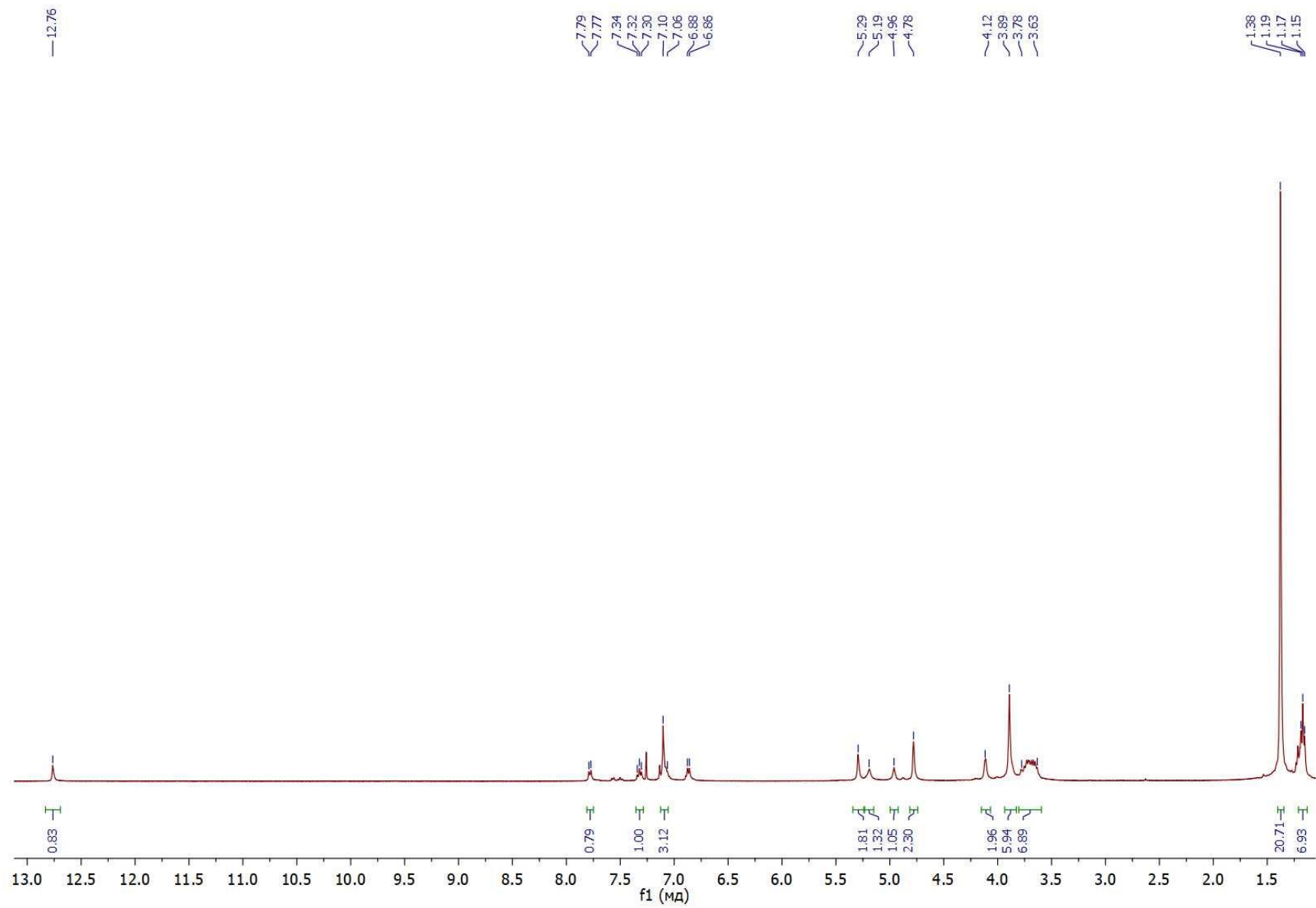


Figure S46. ¹H NMR spectrum of compound **3e** (400 MHz, CDCl₃)

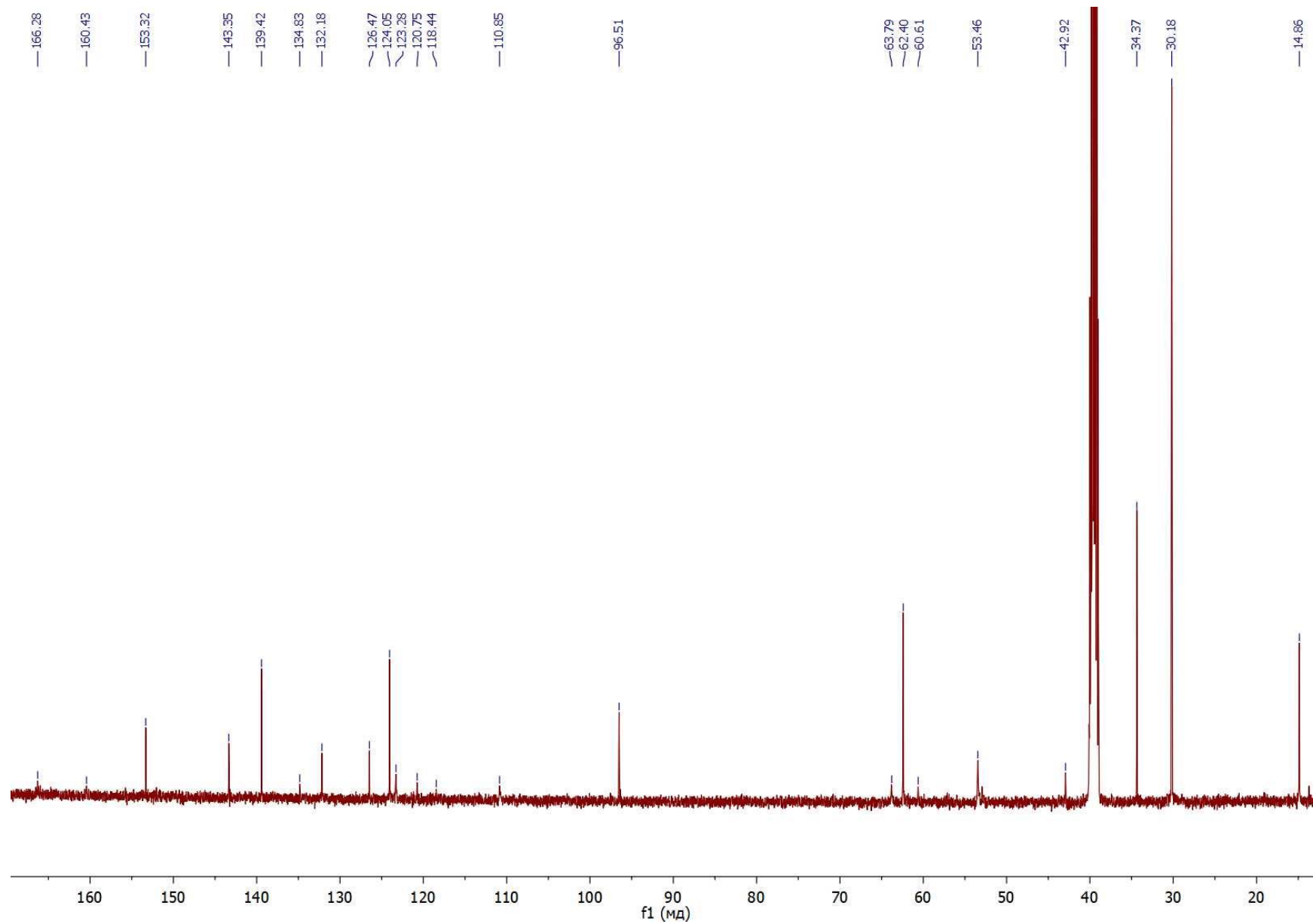


Figure S47. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **3e** (101 MHz, $\text{DMSO}-d_6$)

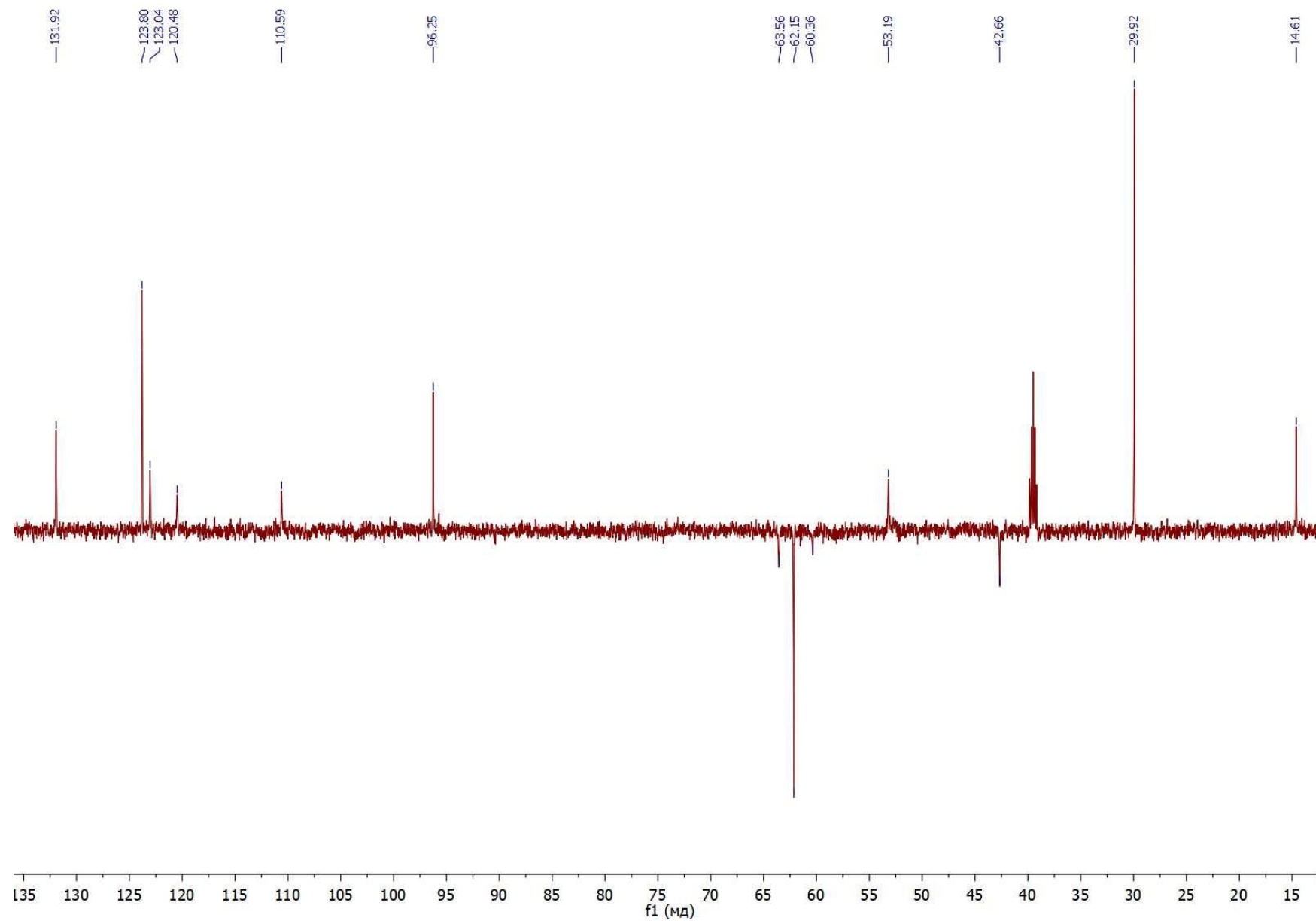


Figure S48. ^{13}C (dept) NMR spectrum of compound **3e** (101 MHz, DMSO- d_6)

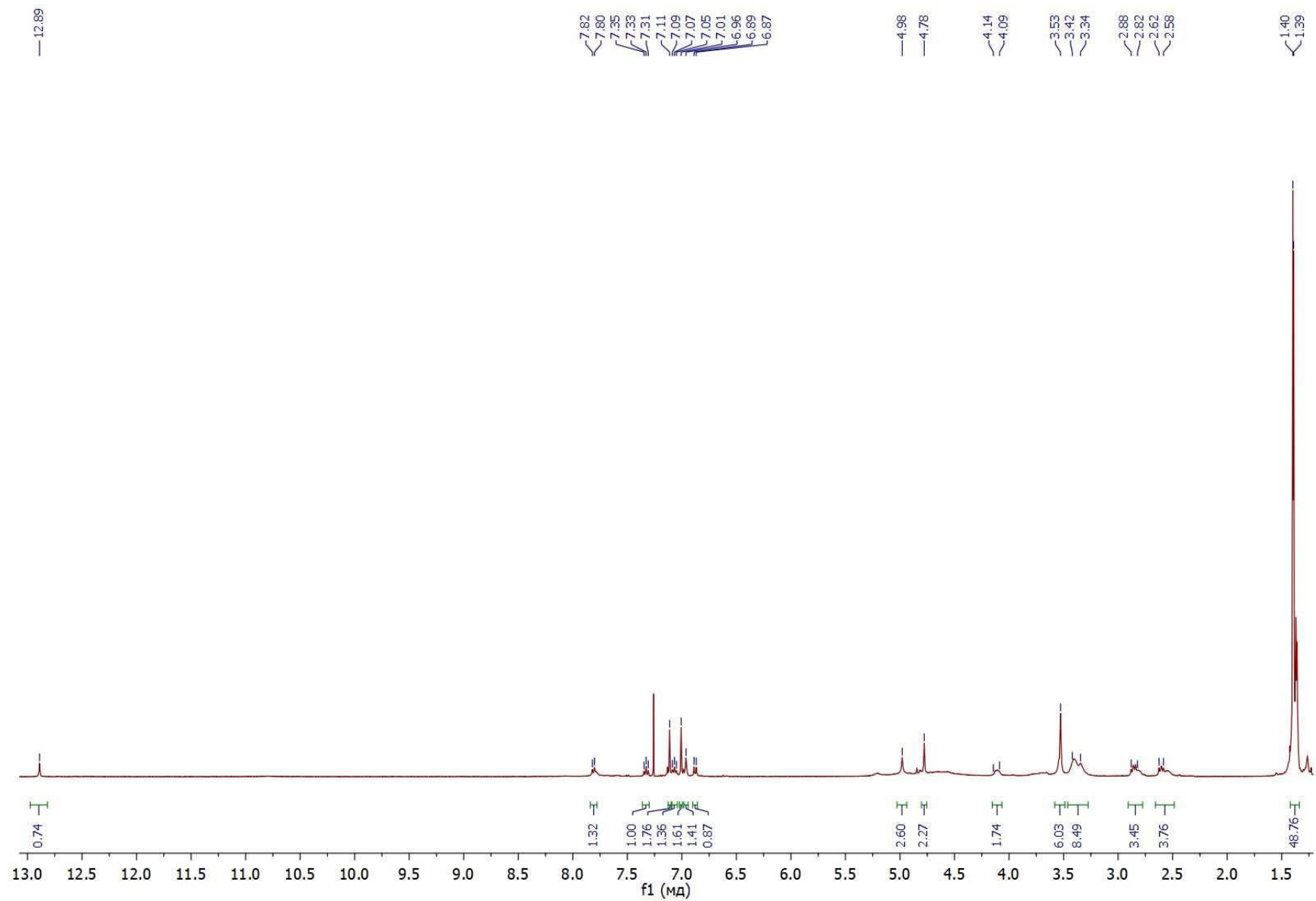


Figure S49. ¹H NMR spectrum of compound **3f** (400 MHz, CDCl₃)

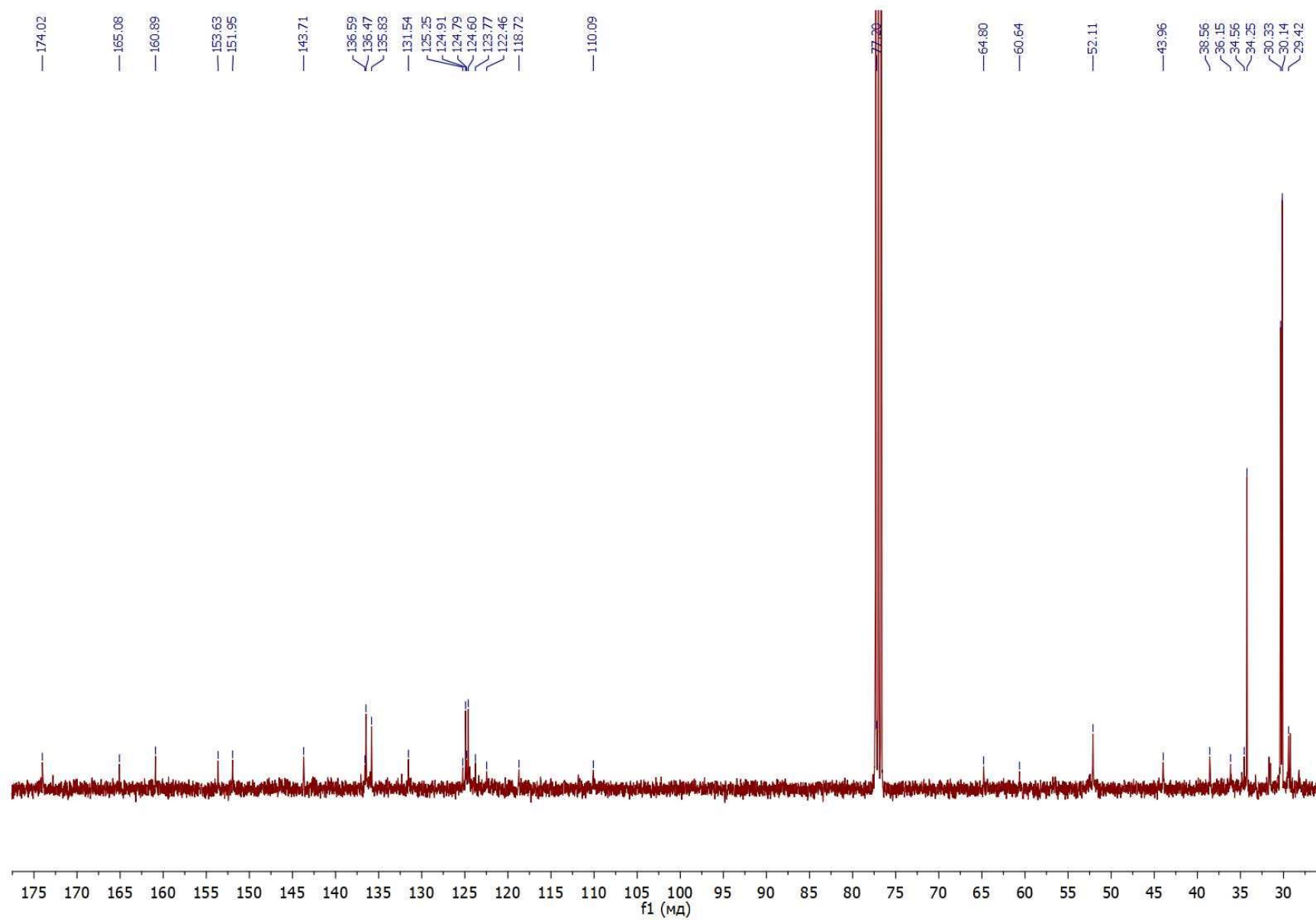


Figure S50. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **3f** (101 MHz, CDCl_3)

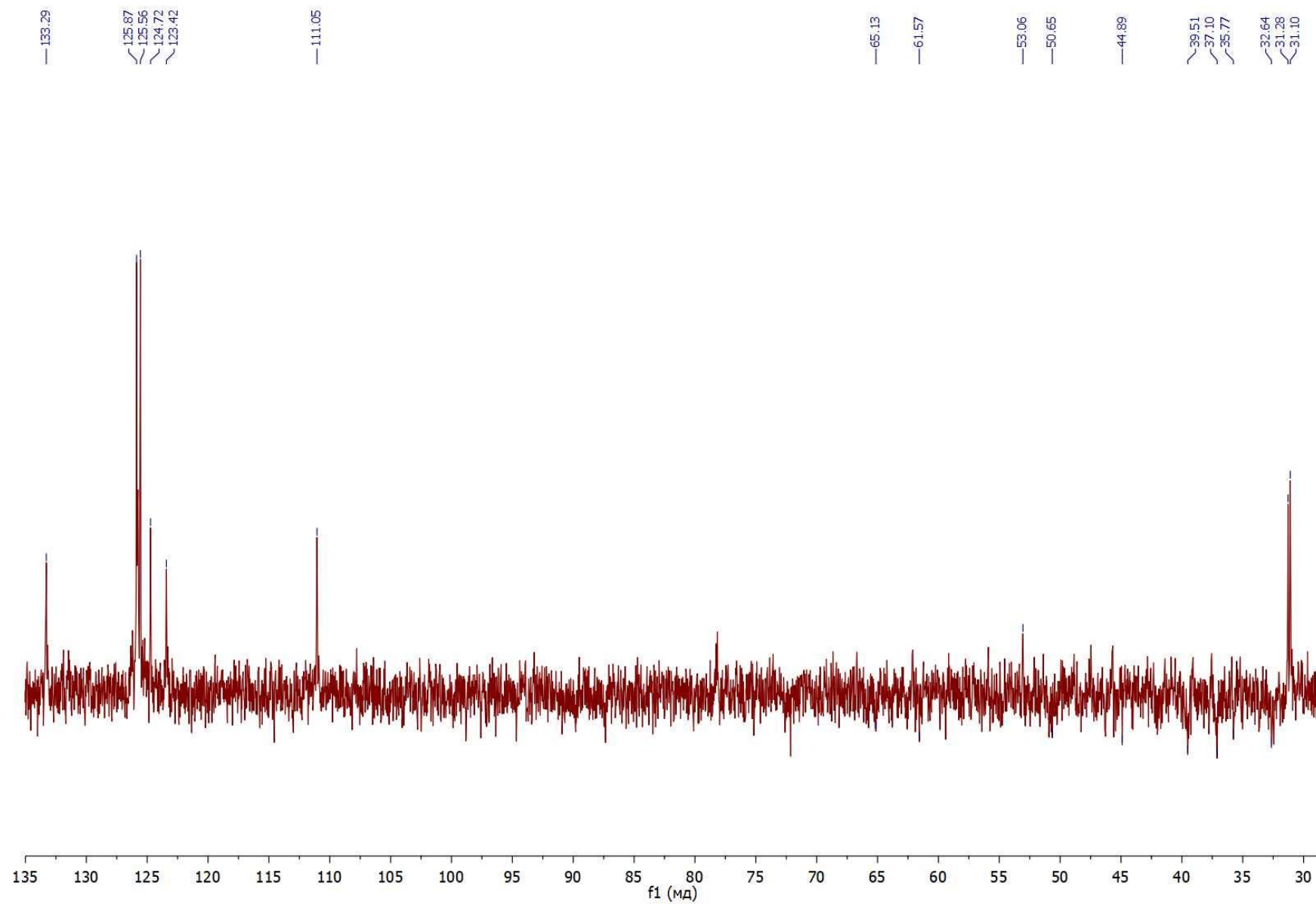


Figure S51. ^{13}C (dept) NMR spectrum of compound **3f** (101 MHz, $CDCl_3$)

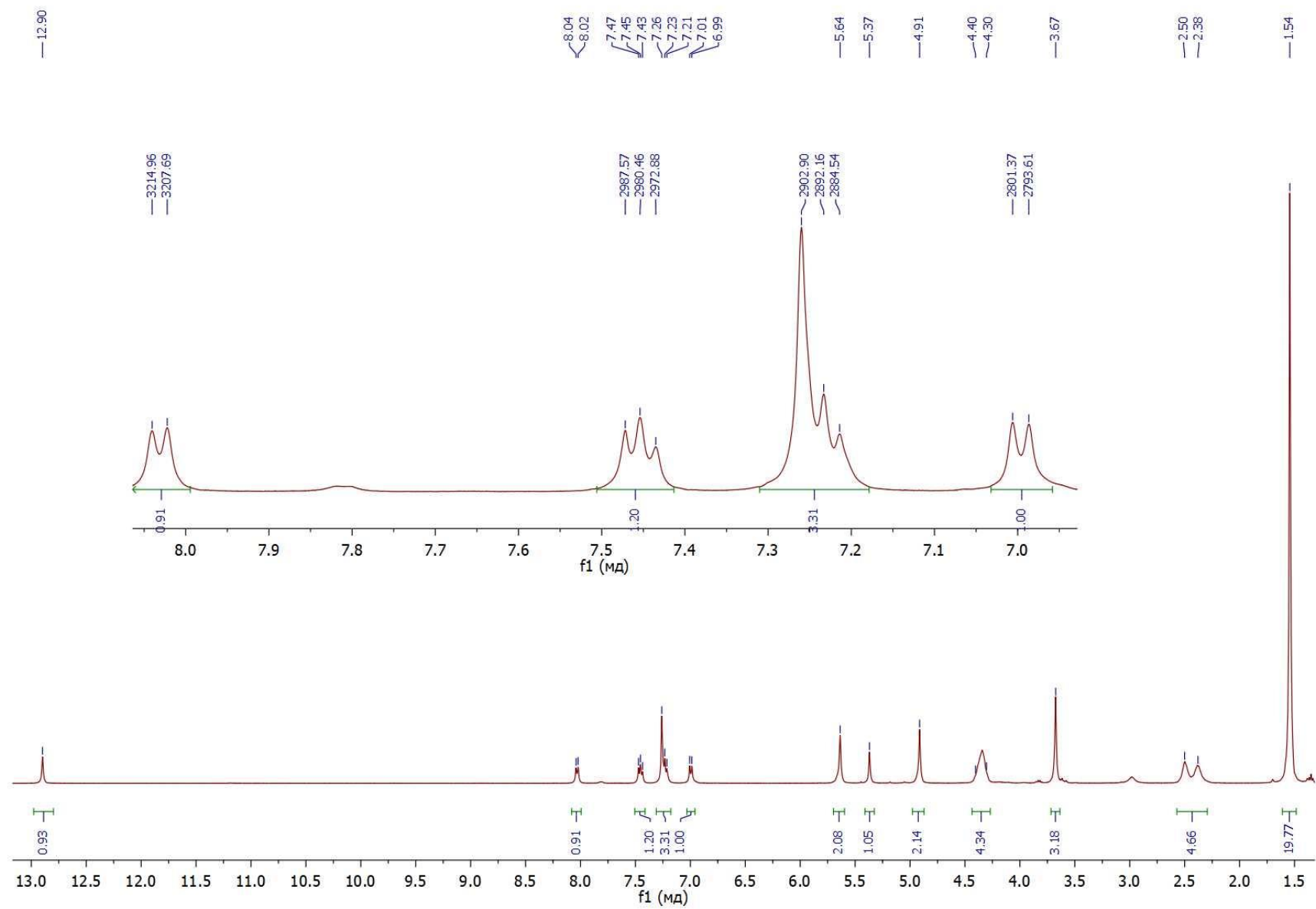


Figure S52. ¹H NMR spectrum of compound **3g** (400 MHz, CDCl₃)

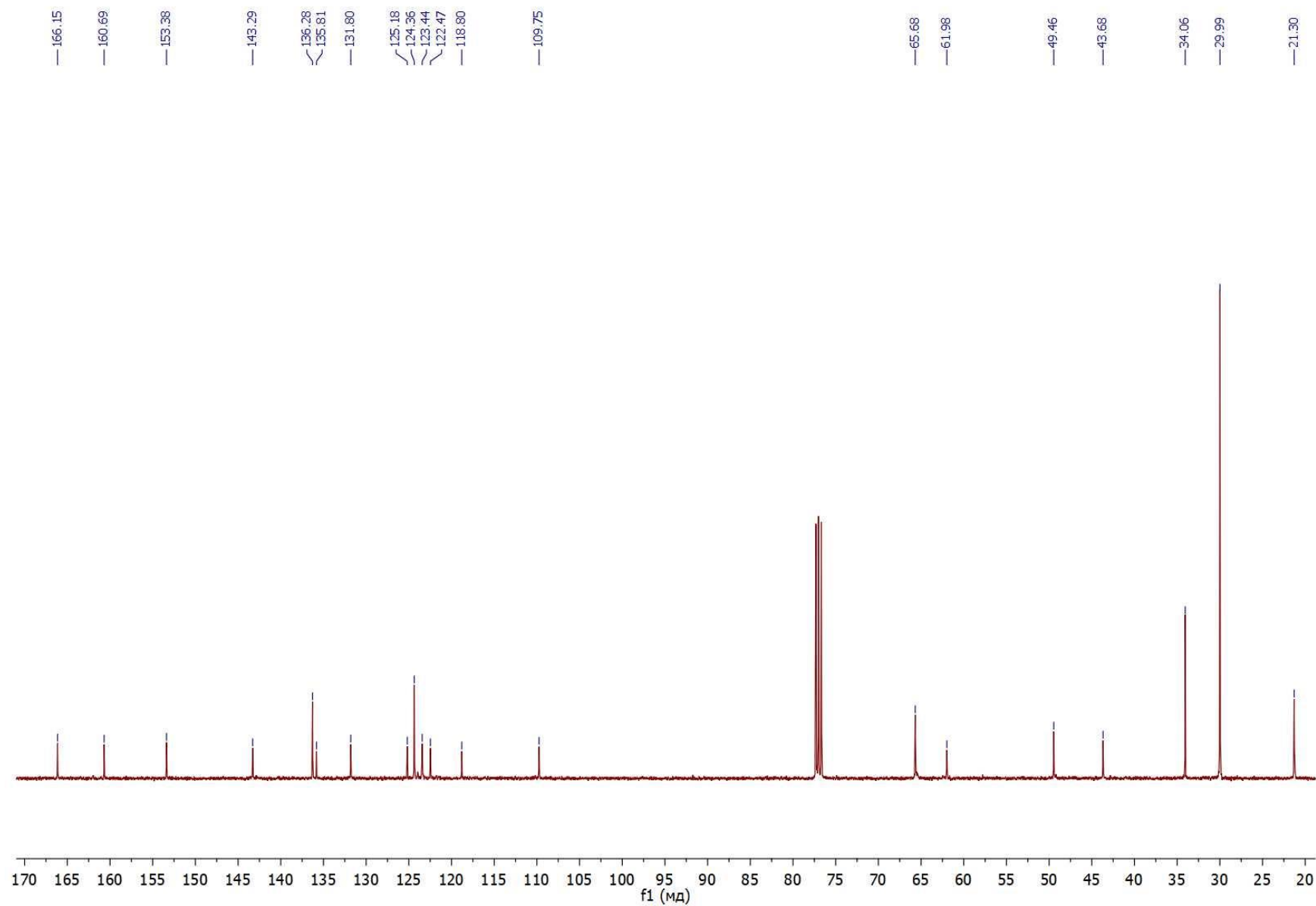


Figure S53. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **3g** (101 MHz, CDCl_3)

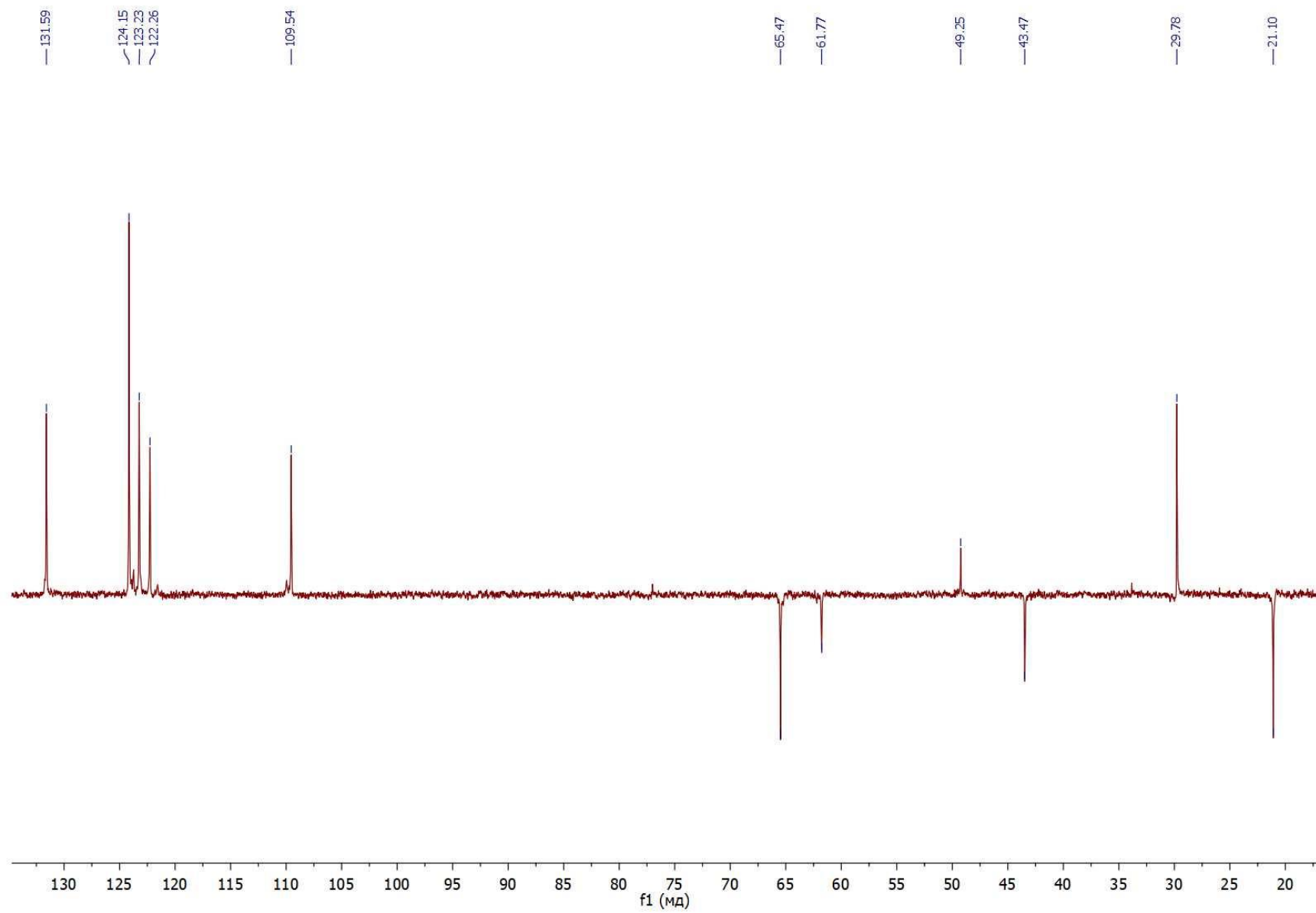


Figure S54. ¹³C (dept) NMR spectrum of compound **3g** (101 MHz, CDCl₃)

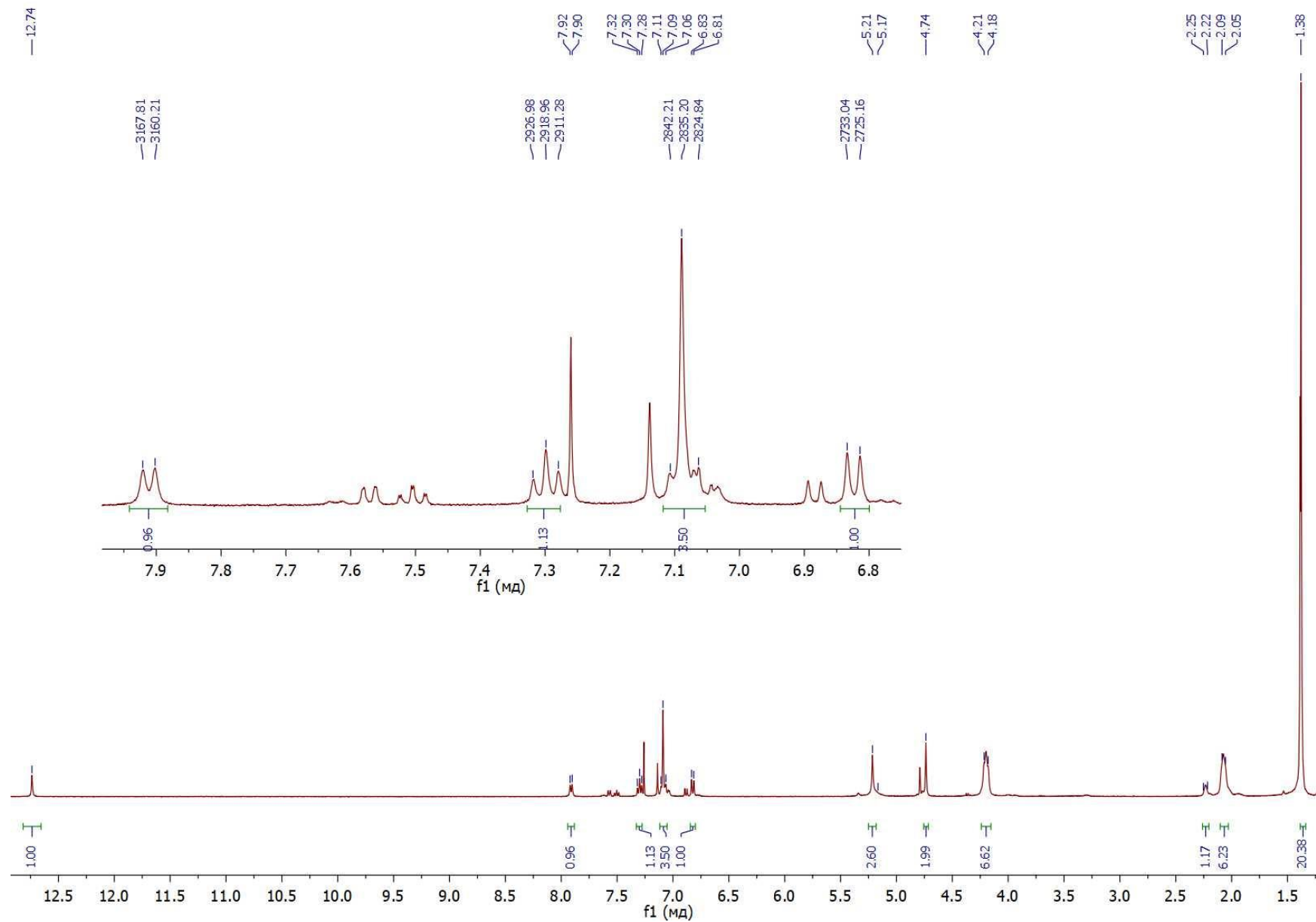


Figure S55. ^1H NMR spectrum of compound **3h** (400 MHz, CDCl_3)

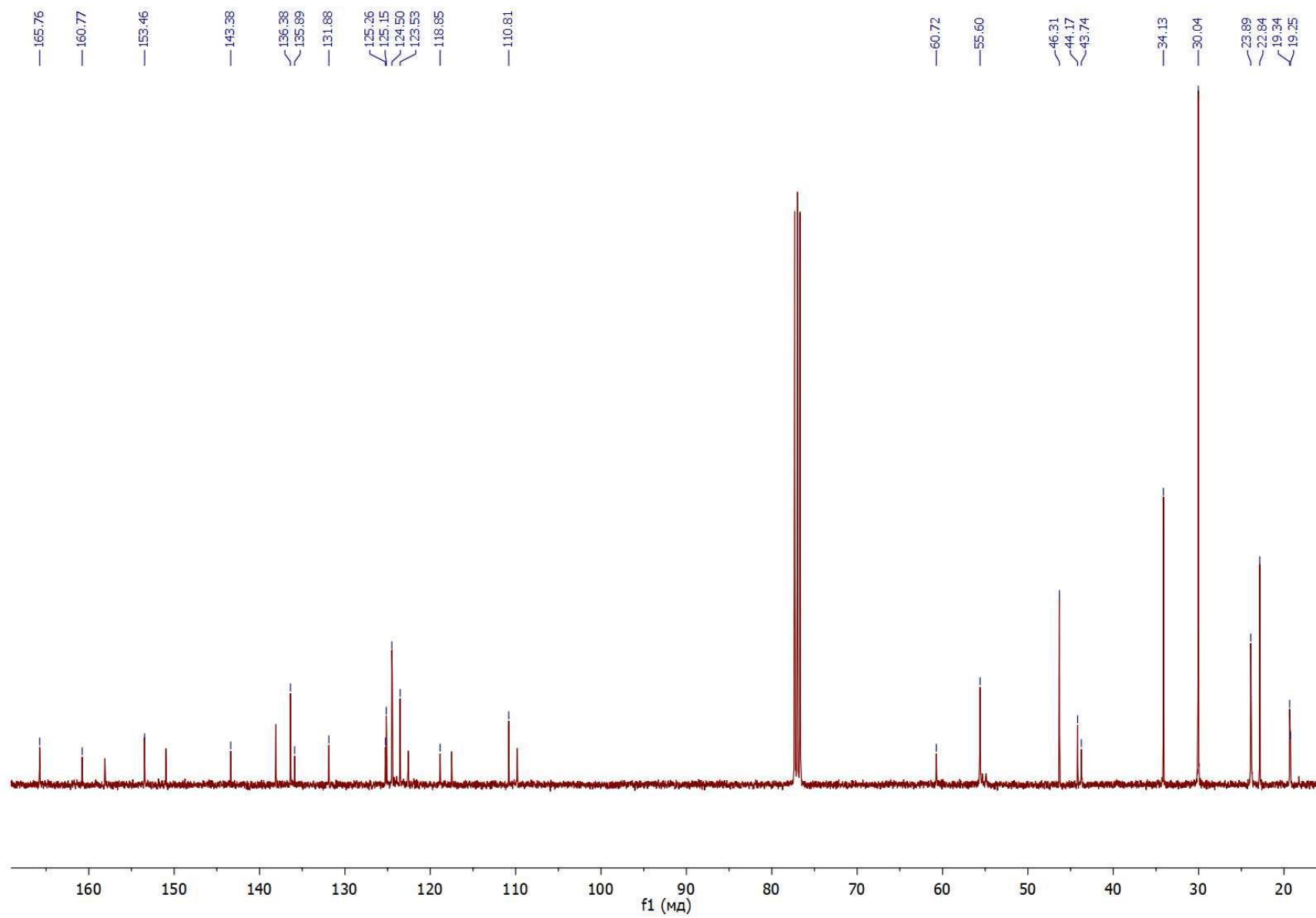


Figure S56. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **3h** (101 MHz, CDCl_3)

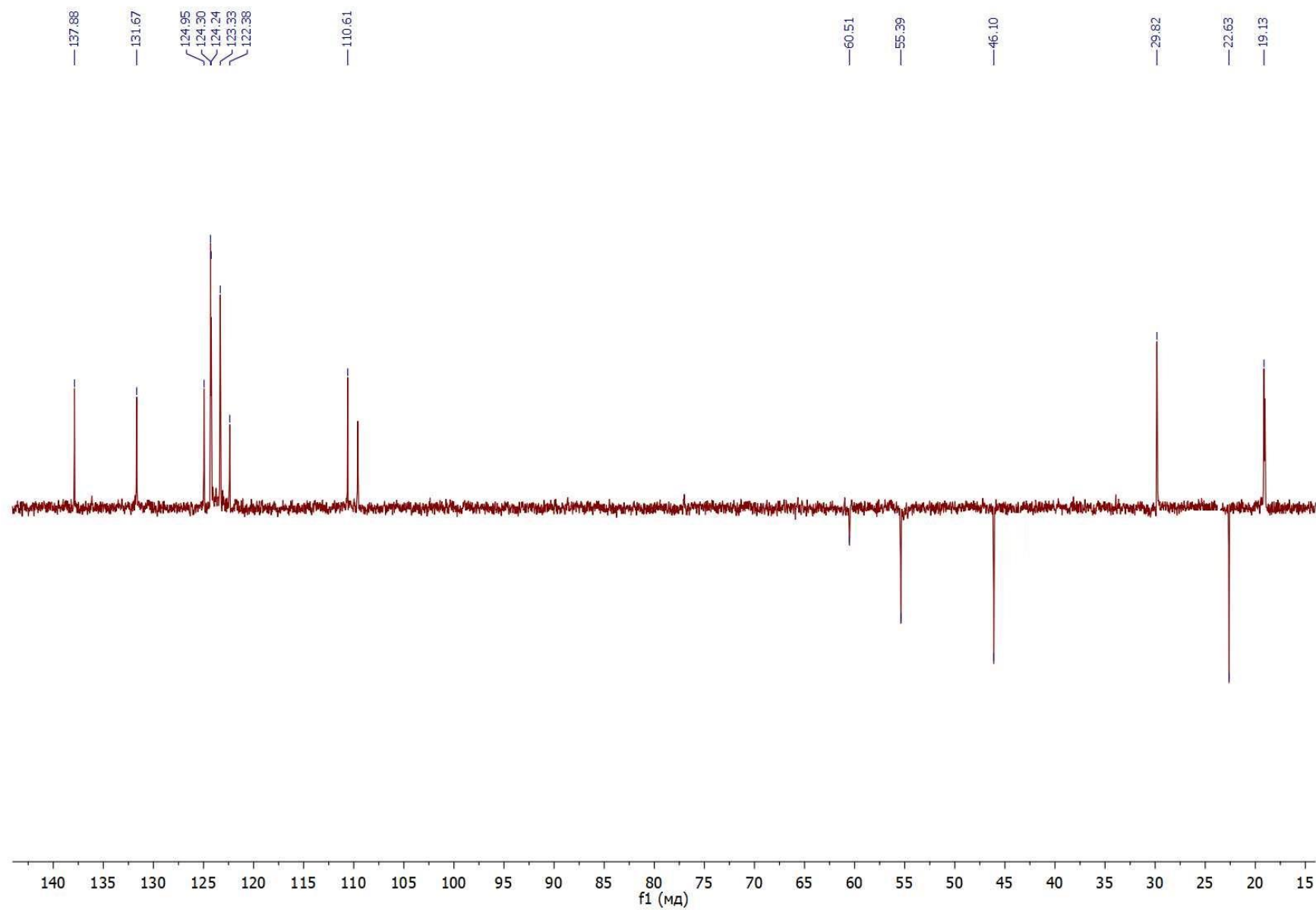


Figure S57. ^{13}C (dept) NMR spectrum of compound **3h** (101 MHz, CDCl_3)

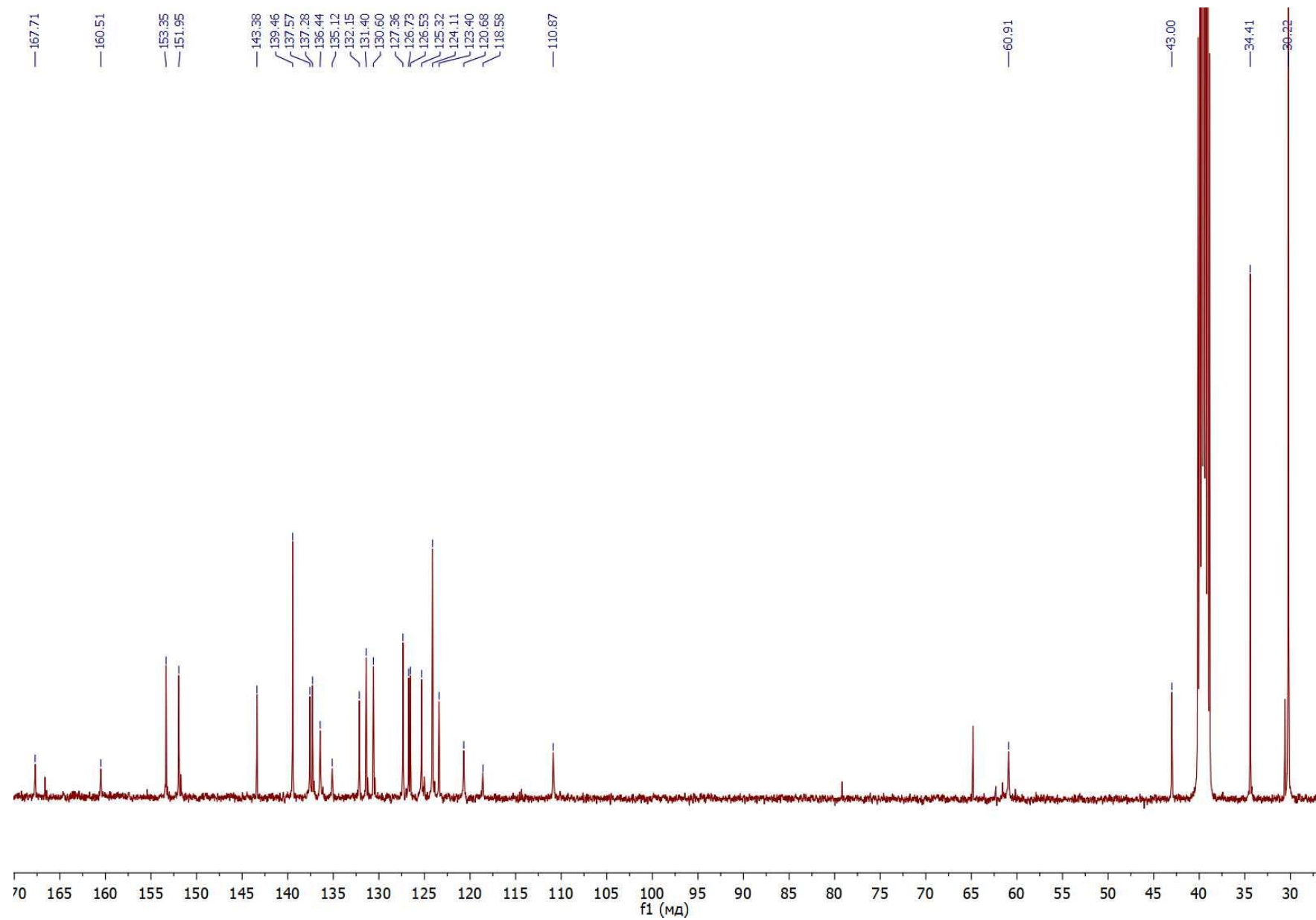


Figure S59. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **3i** (101 MHz, $\text{DMSO-}d_6$)

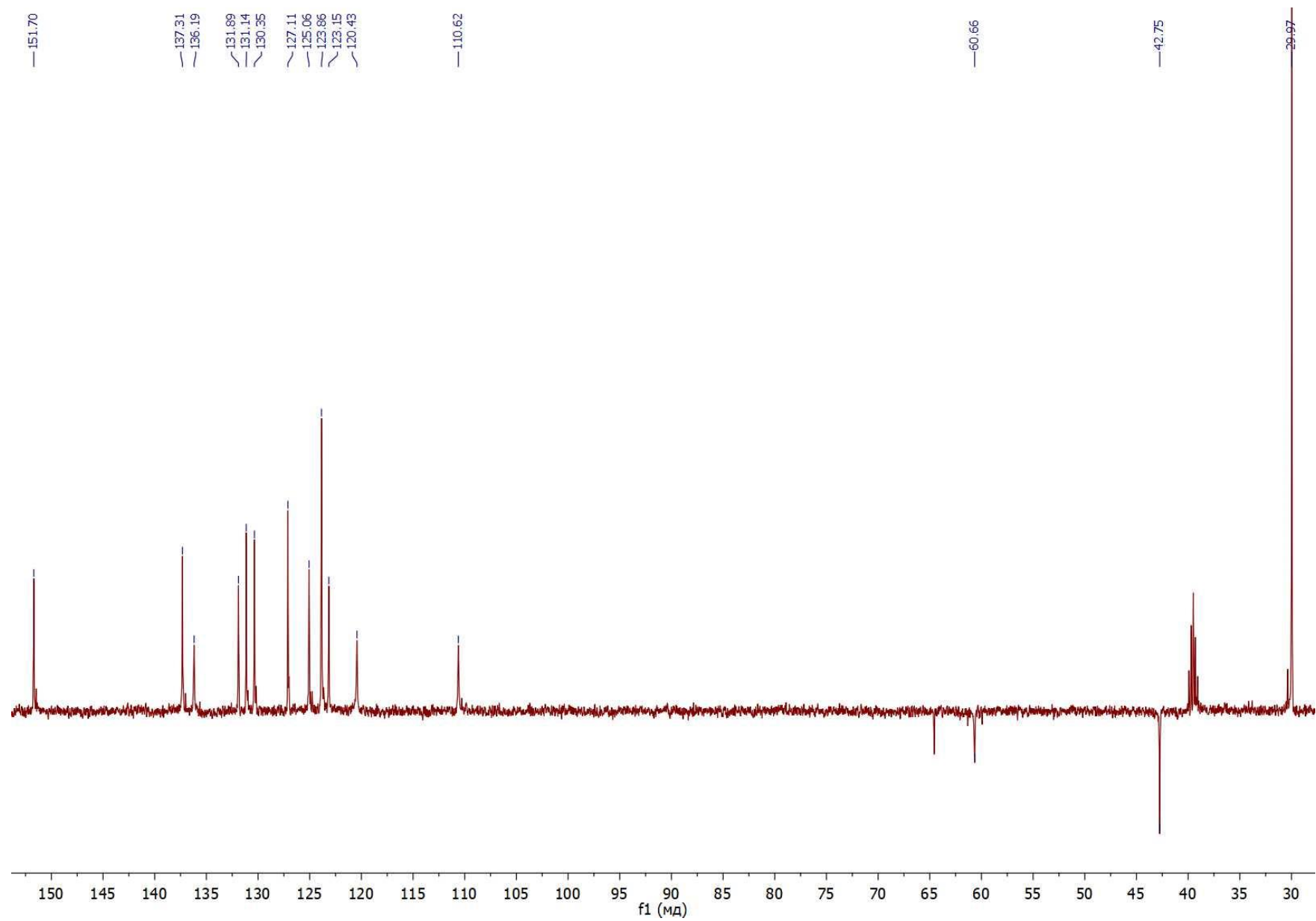


Figure S60. ^{13}C (dept) NMR spectrum of compound **3i** (101 MHz, DMSO- d_6)

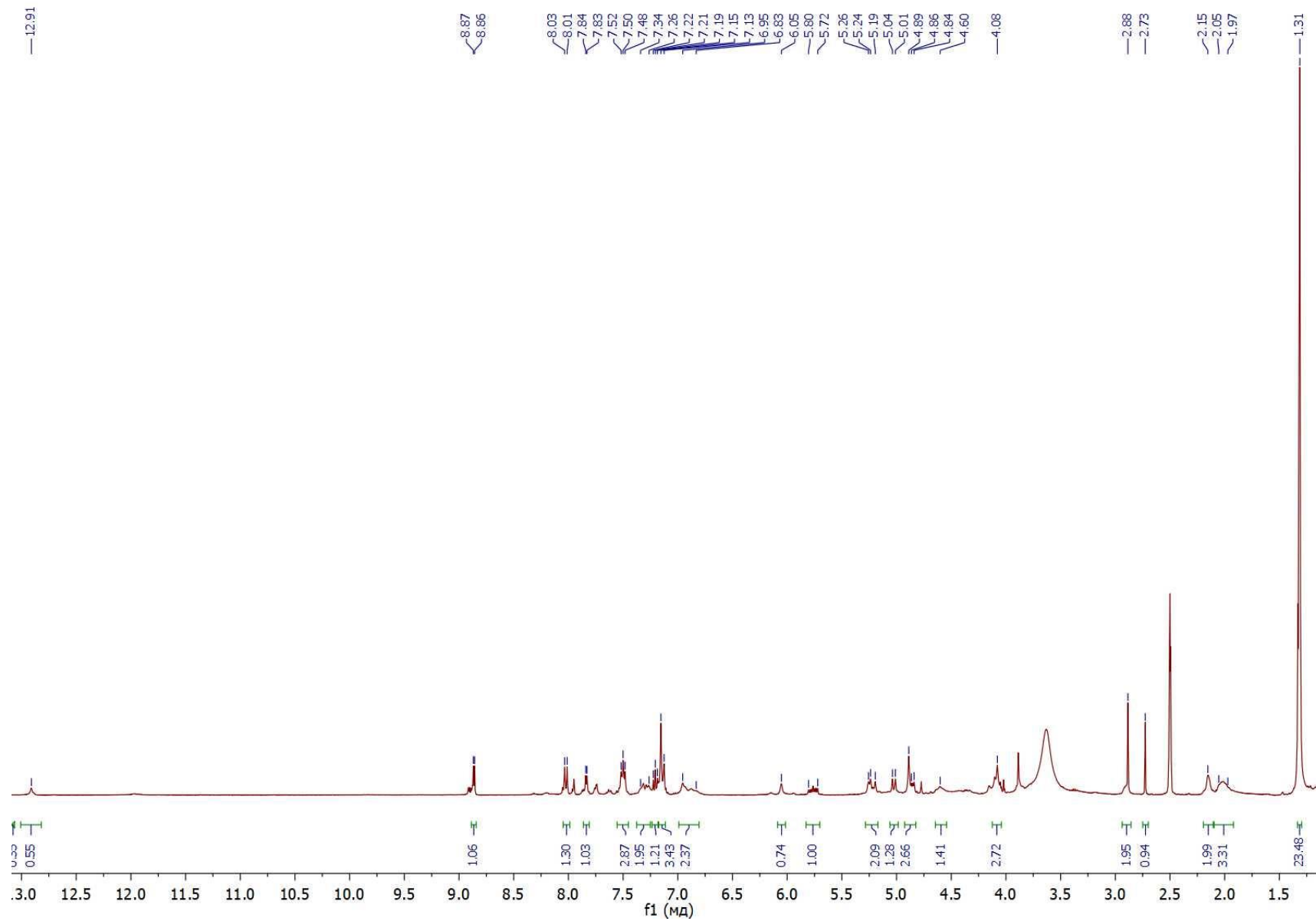


Figure S61. ^1H NMR spectrum of compound **3j** (400 MHz, $\text{DMSO}-d_6$)

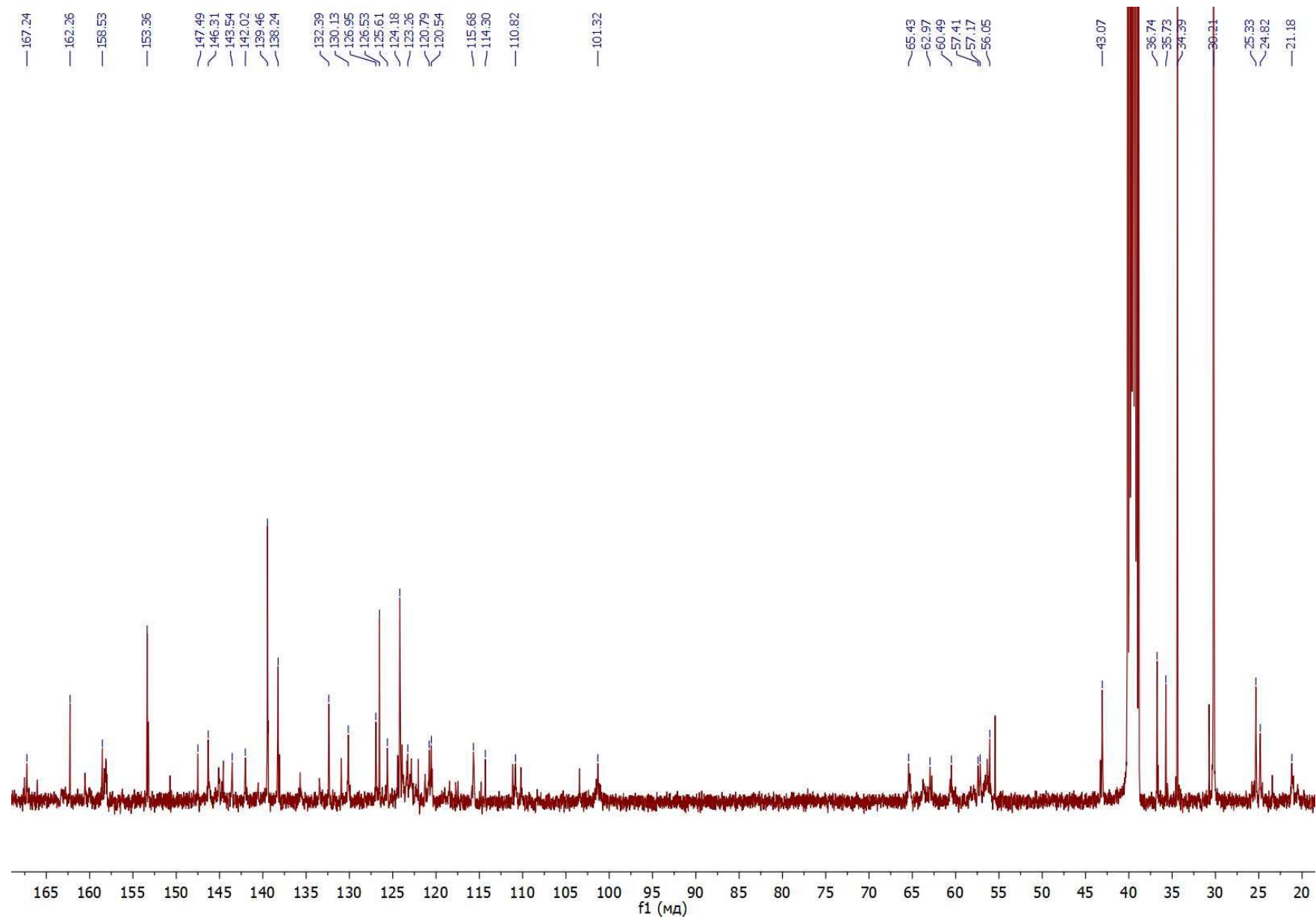


Figure S62. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **3j** (101 MHz, $\text{DMSO}-d_6$)

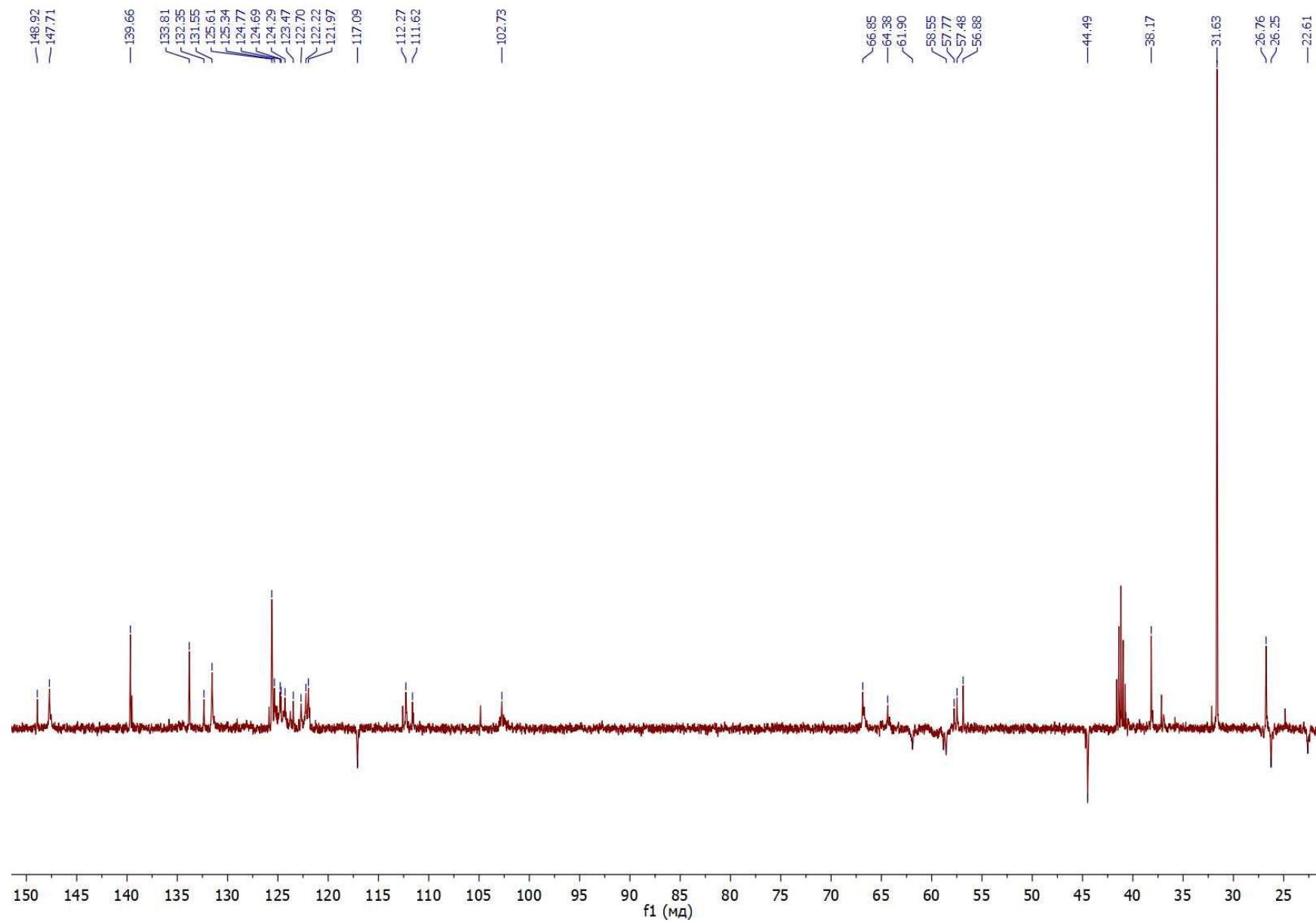


Figure S63. ^{13}C (dept) NMR spectrum of compound **3j** (101 MHz, $\text{DMSO}-d_6$)

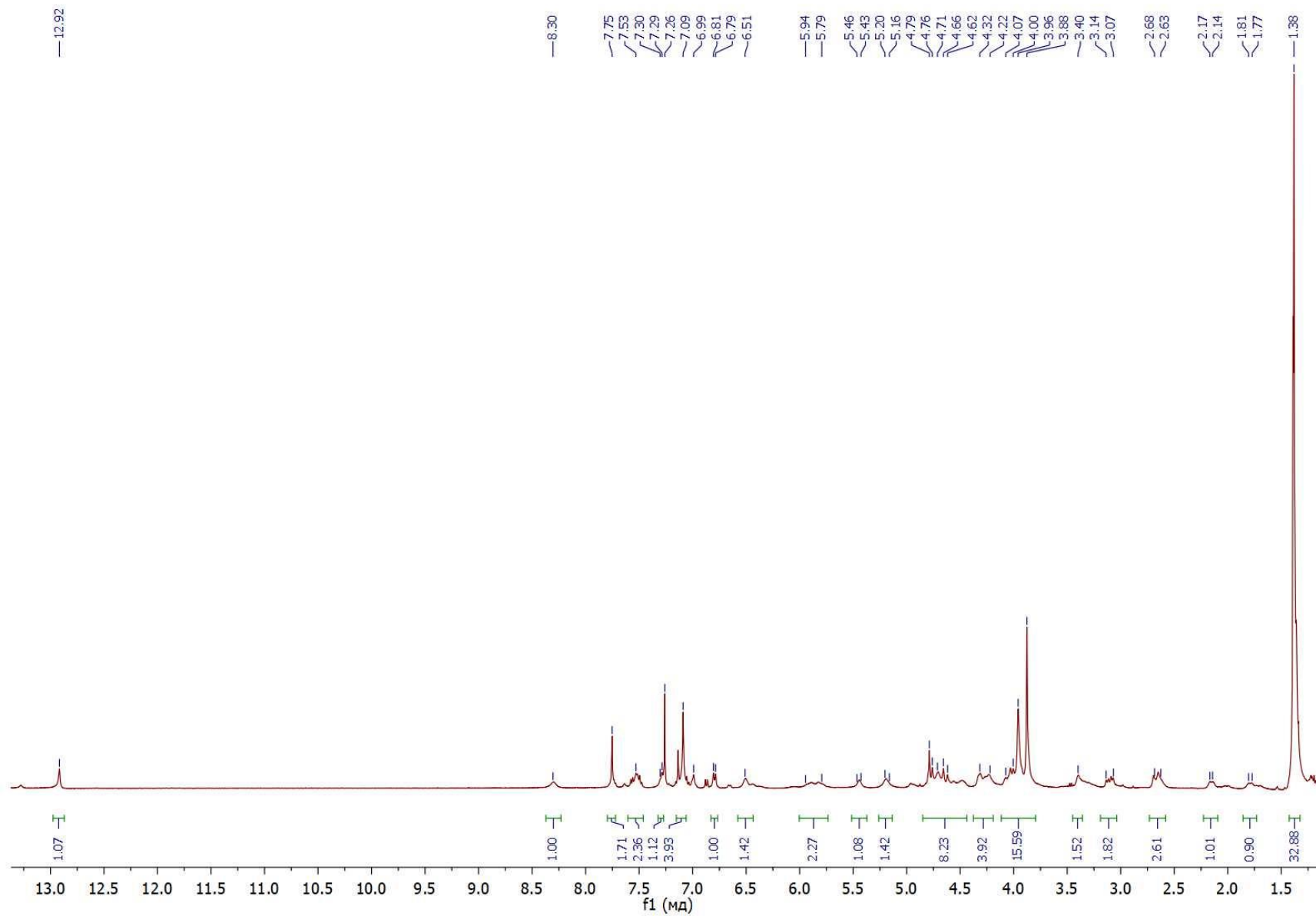


Figure S64. ¹H NMR spectrum of compound **3k** (400 MHz, CDCl₃)

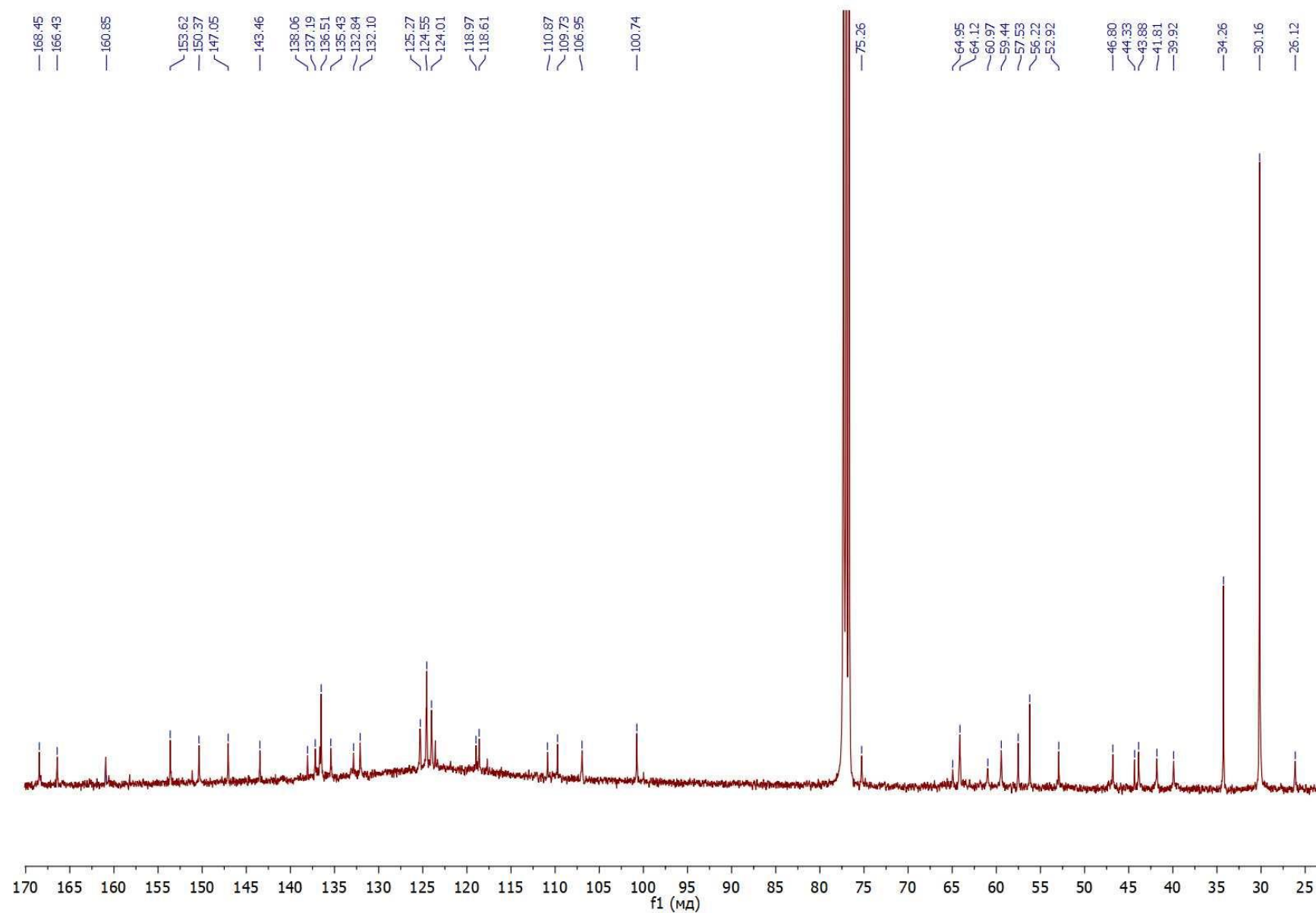


Figure S65. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **3k** (101 MHz, CDCl_3)

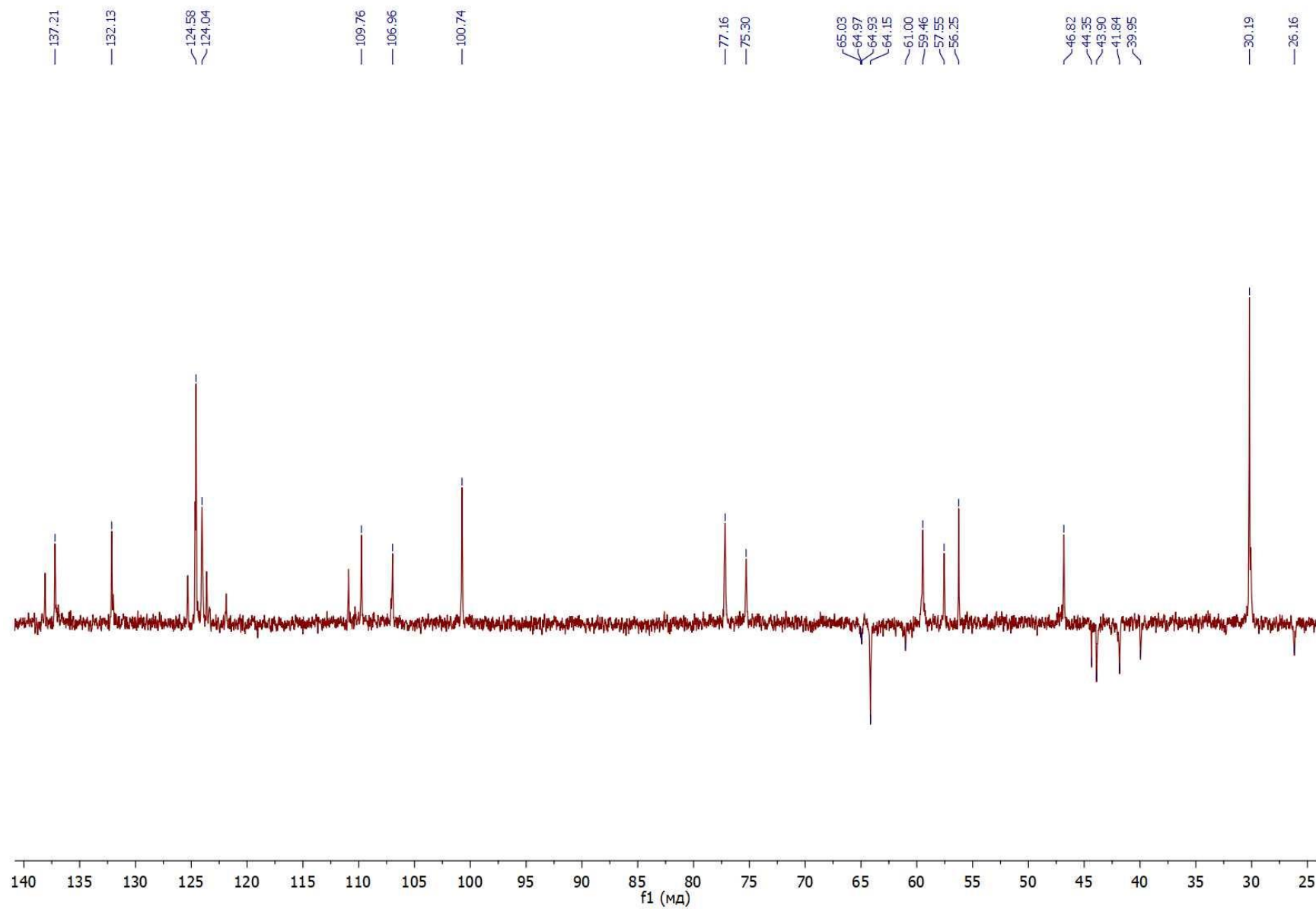


Figure S66. ^{13}C (dept) NMR spectrum of compound **3k** (101 MHz, CDCl_3)

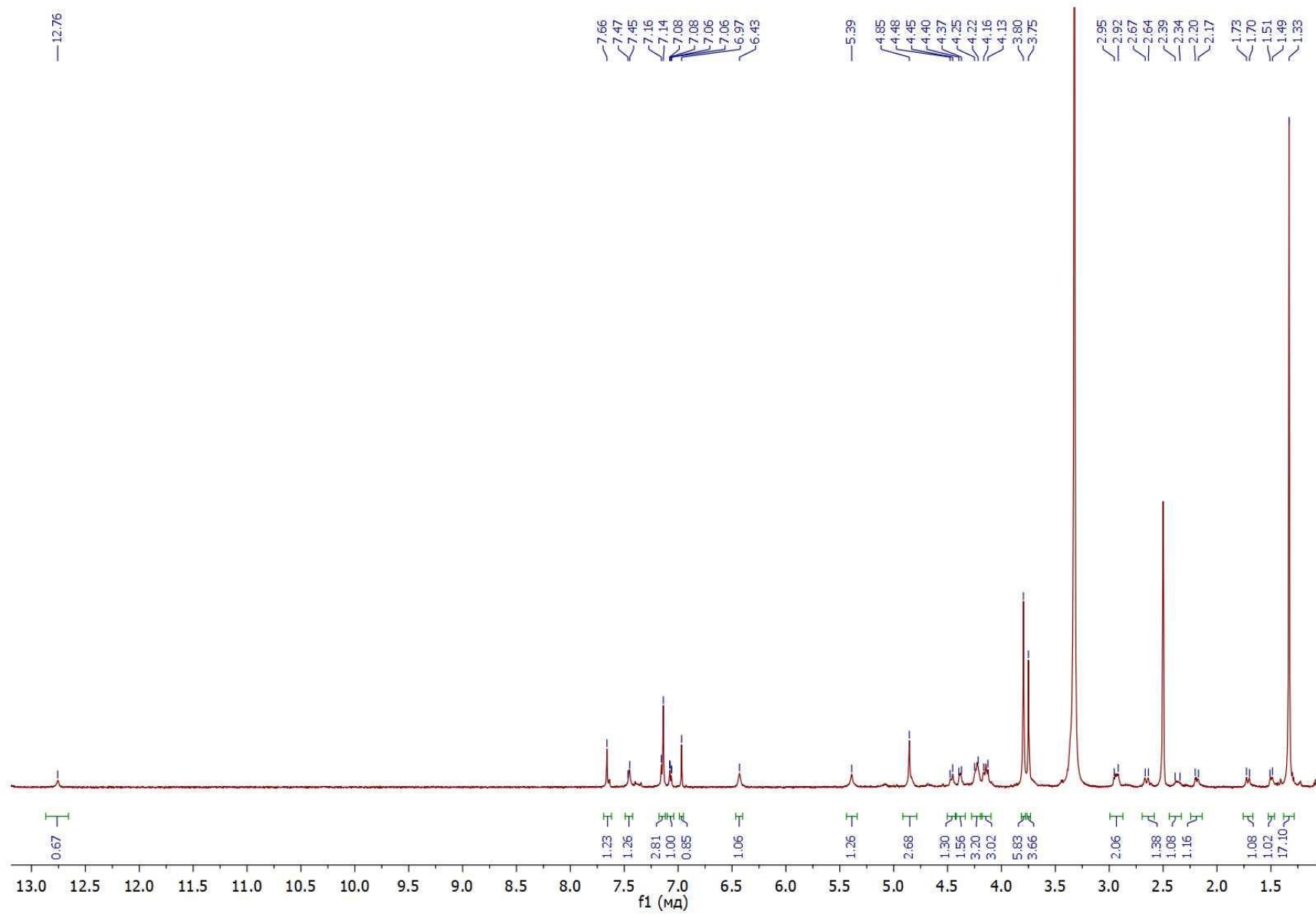


Figure S67. ¹H NMR spectrum of compound **3I** (600 MHz, DMSO-*d*₆)

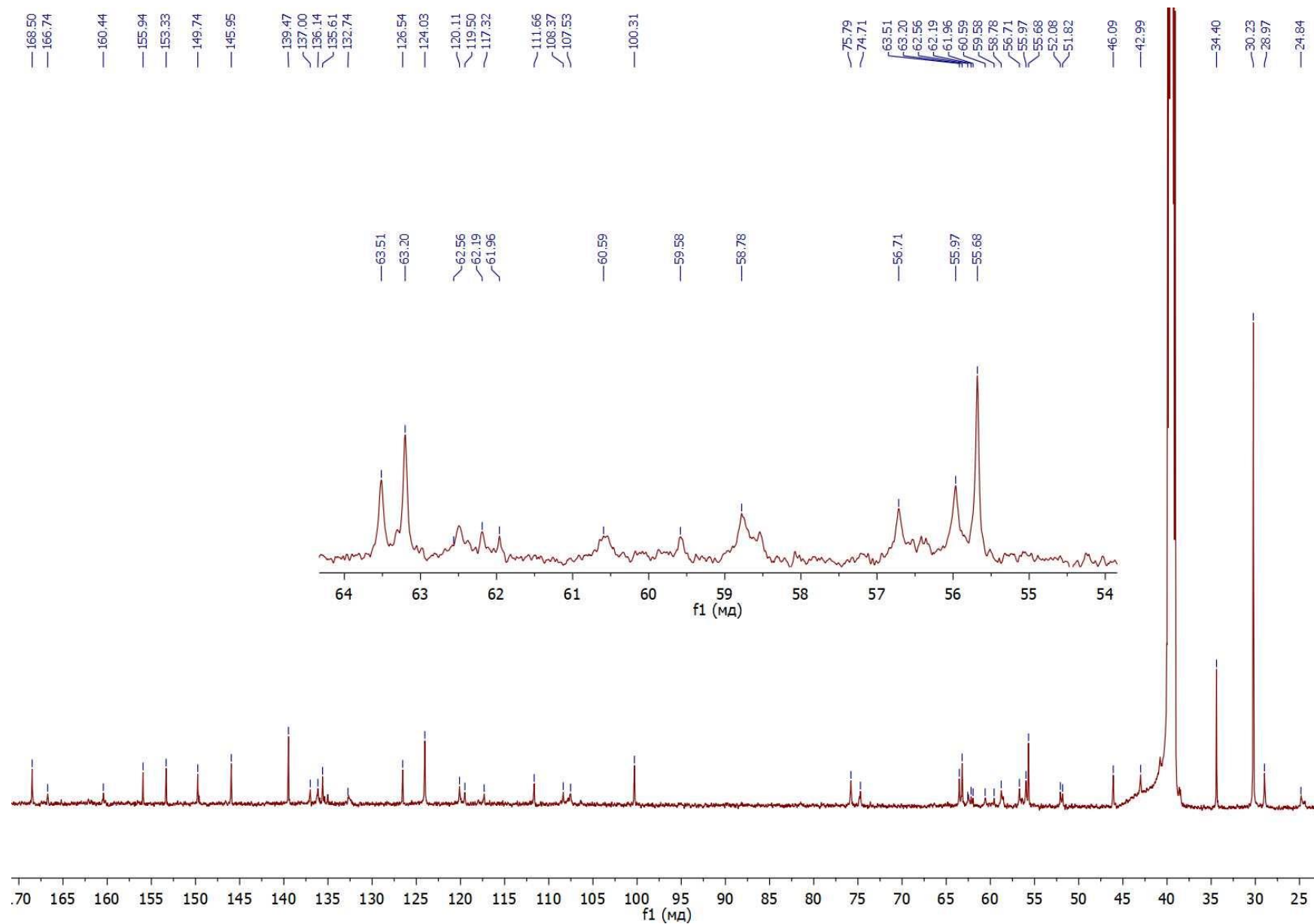


Figure S68. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **3I** (151 MHz, $\text{DMSO}-d_6$)

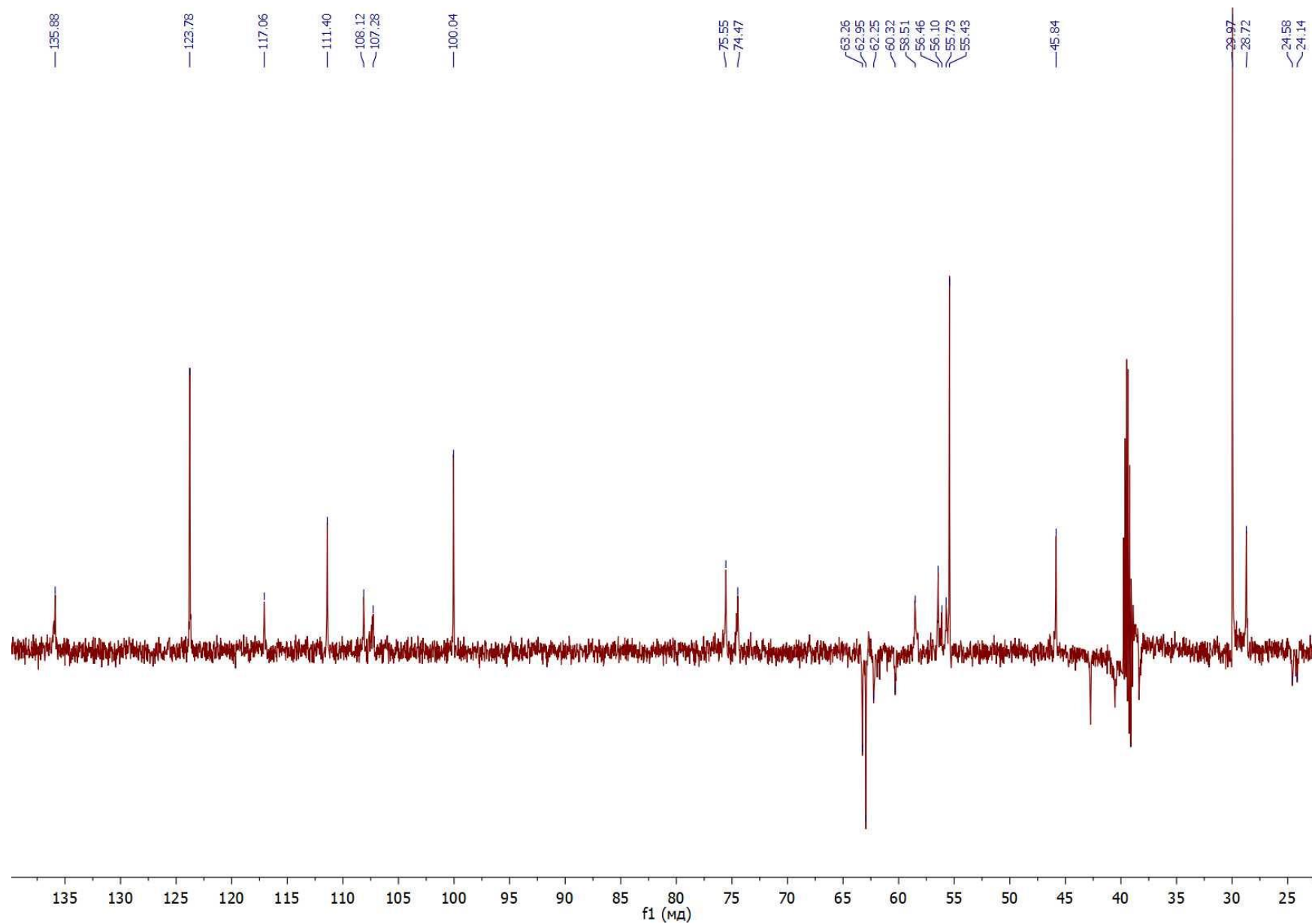


Figure S69. ^{13}C (dept) NMR spectrum of compound **3I** (151 MHz, $\text{DMSO}-d_6$)

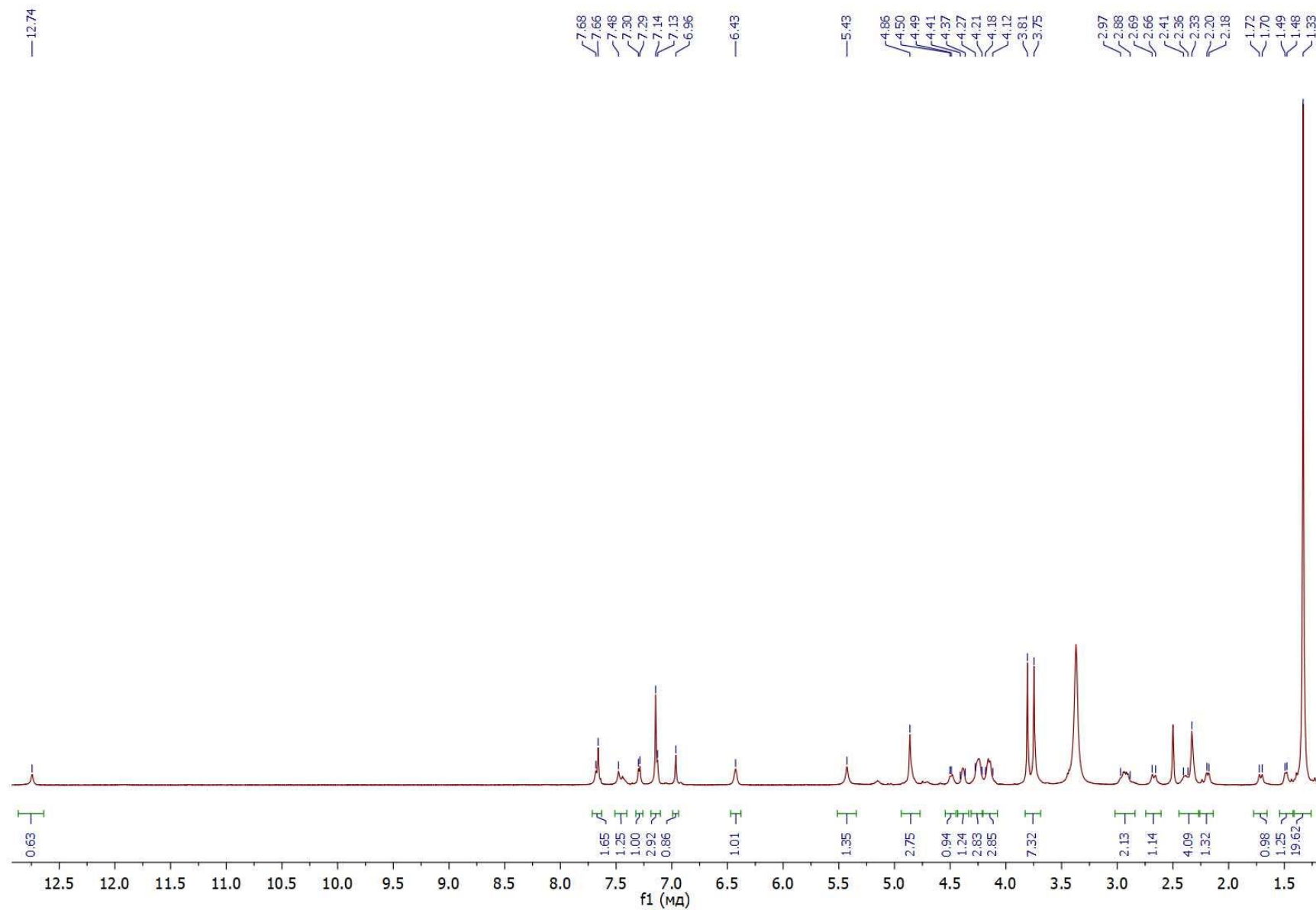


Figure S70. ¹H NMR spectrum of compound **3m** (600 MHz, DMSO-*d*₆)

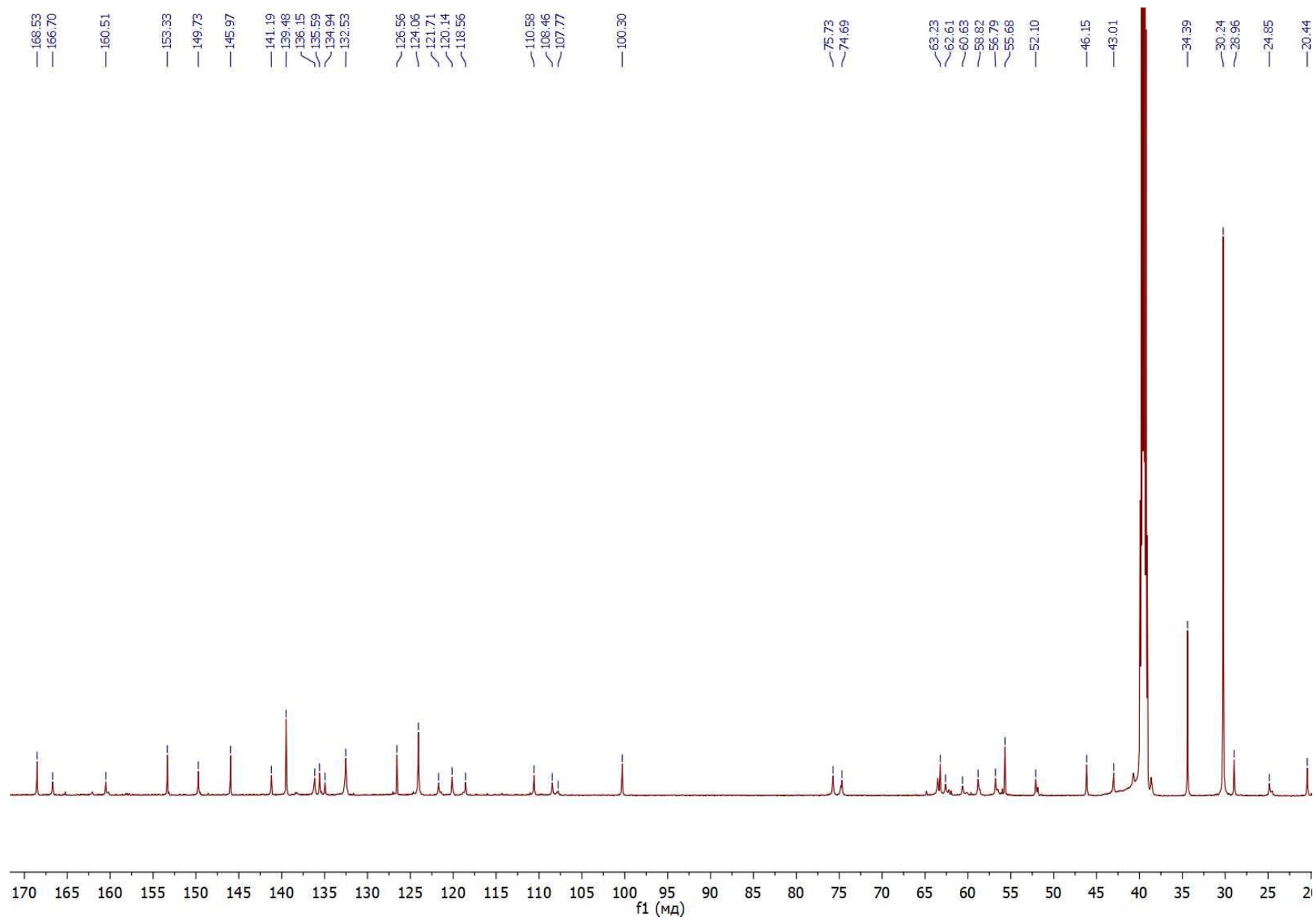


Figure S71. $^{13}\text{C}\{-^1\text{H}\}$ NMR spectrum of compound **3m** (151 MHz, $\text{DMSO}-d_6$)

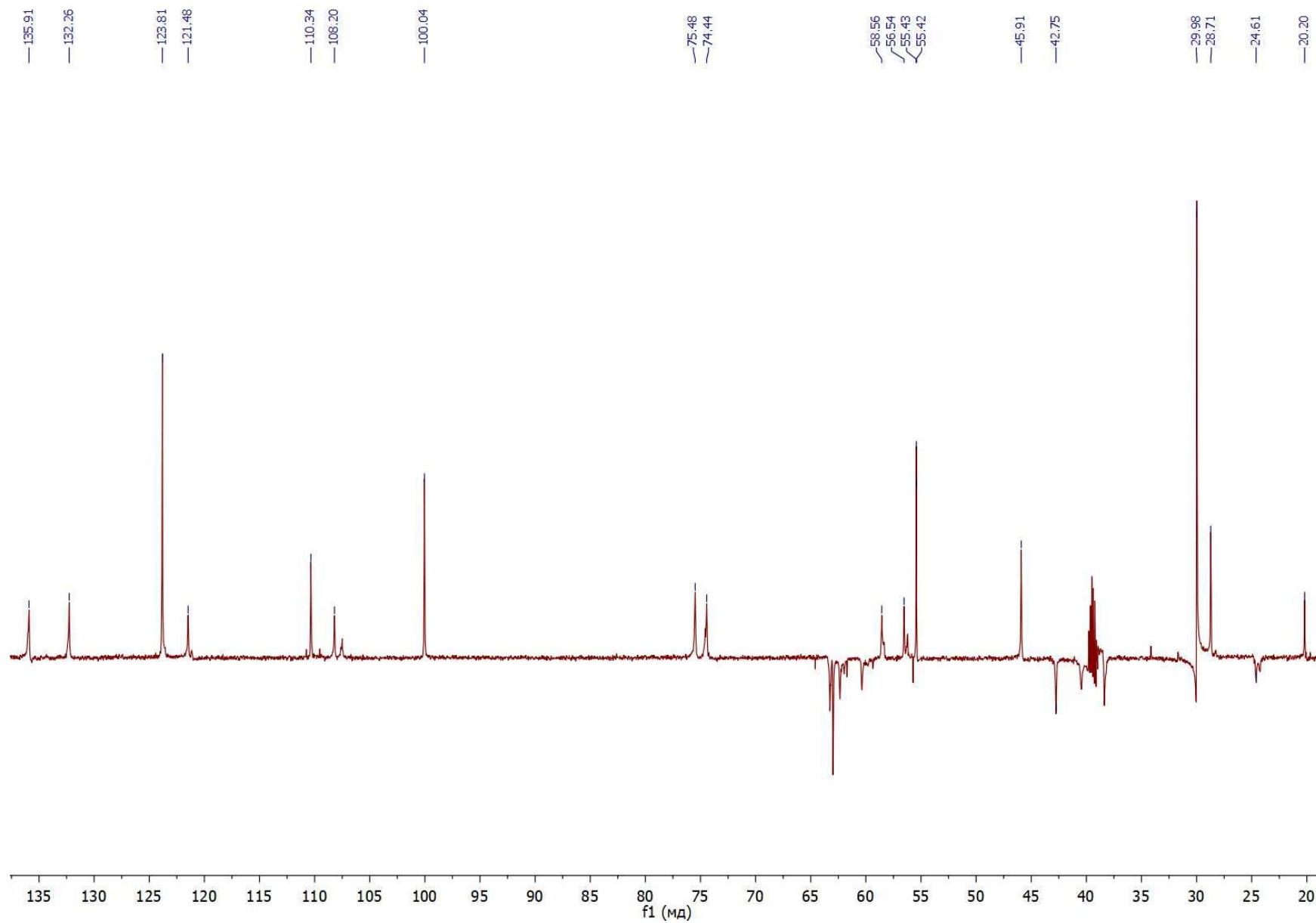


Figure S72. ^{13}C (dept) NMR spectrum of compound **3m** (151 MHz, $\text{DMSO}-d_6$)

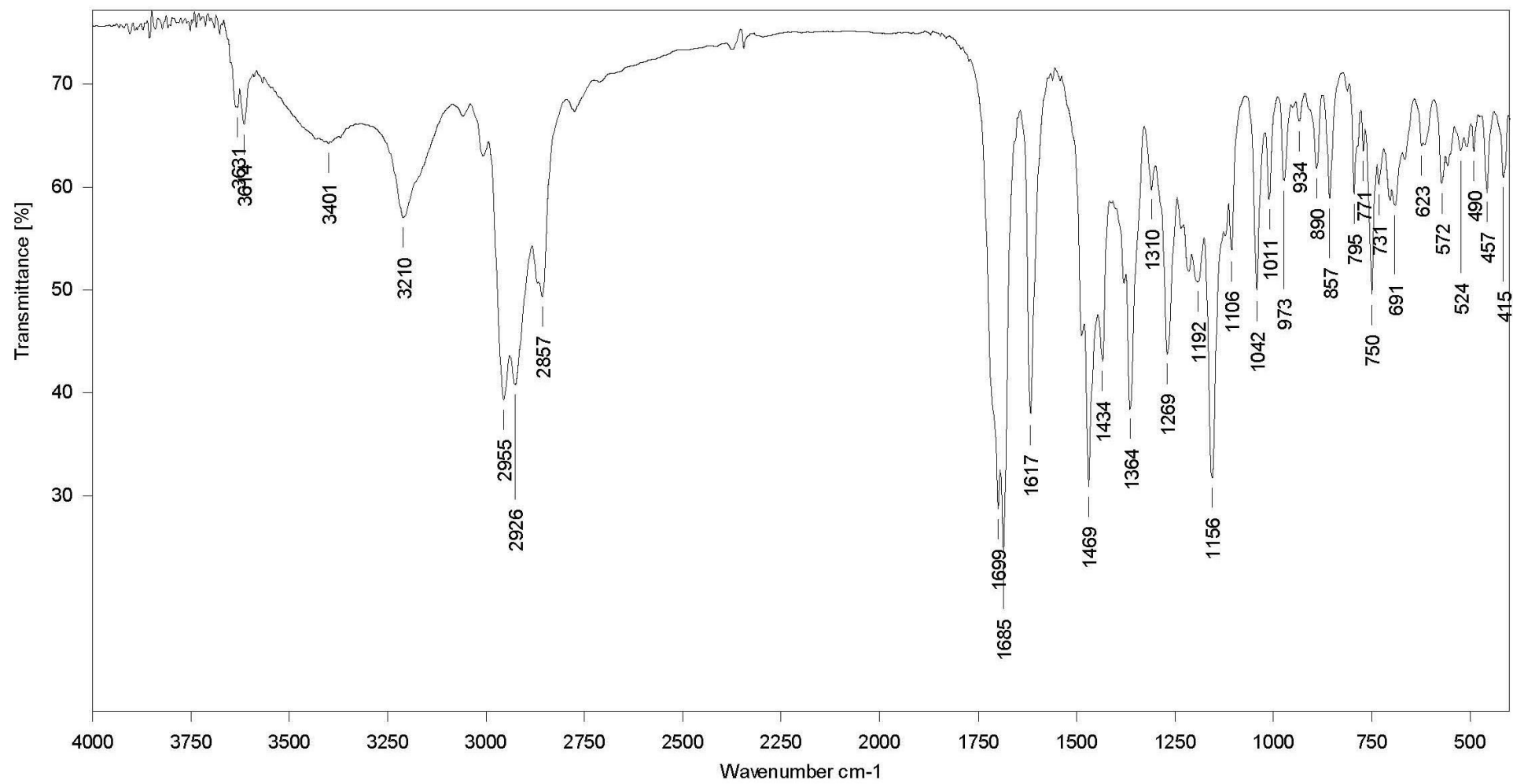


Figure S73. IR spectrum of compound **3a** (in KBr pellet)

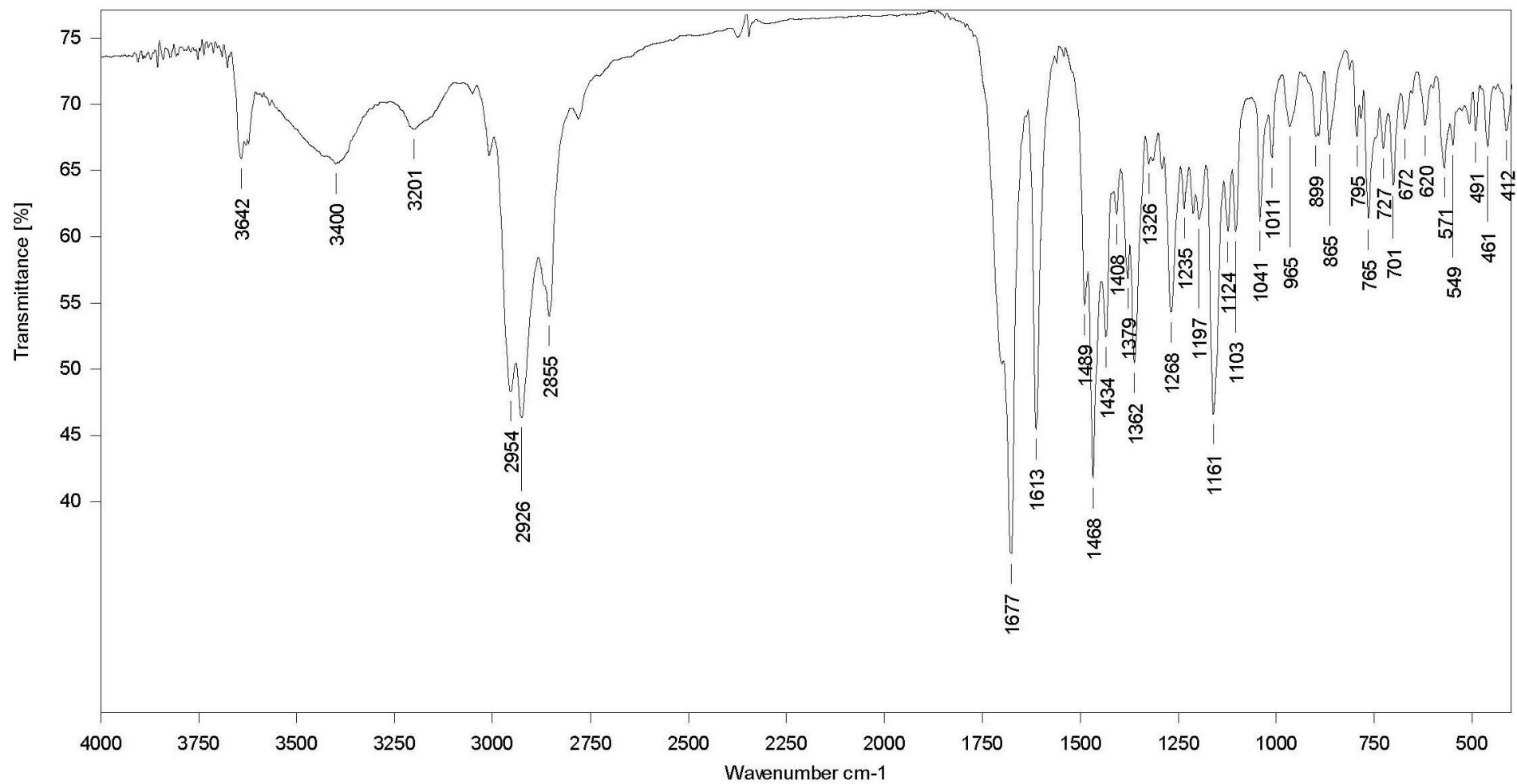


Figure S74. IR spectrum of compound **3b** (in KBr pellet)

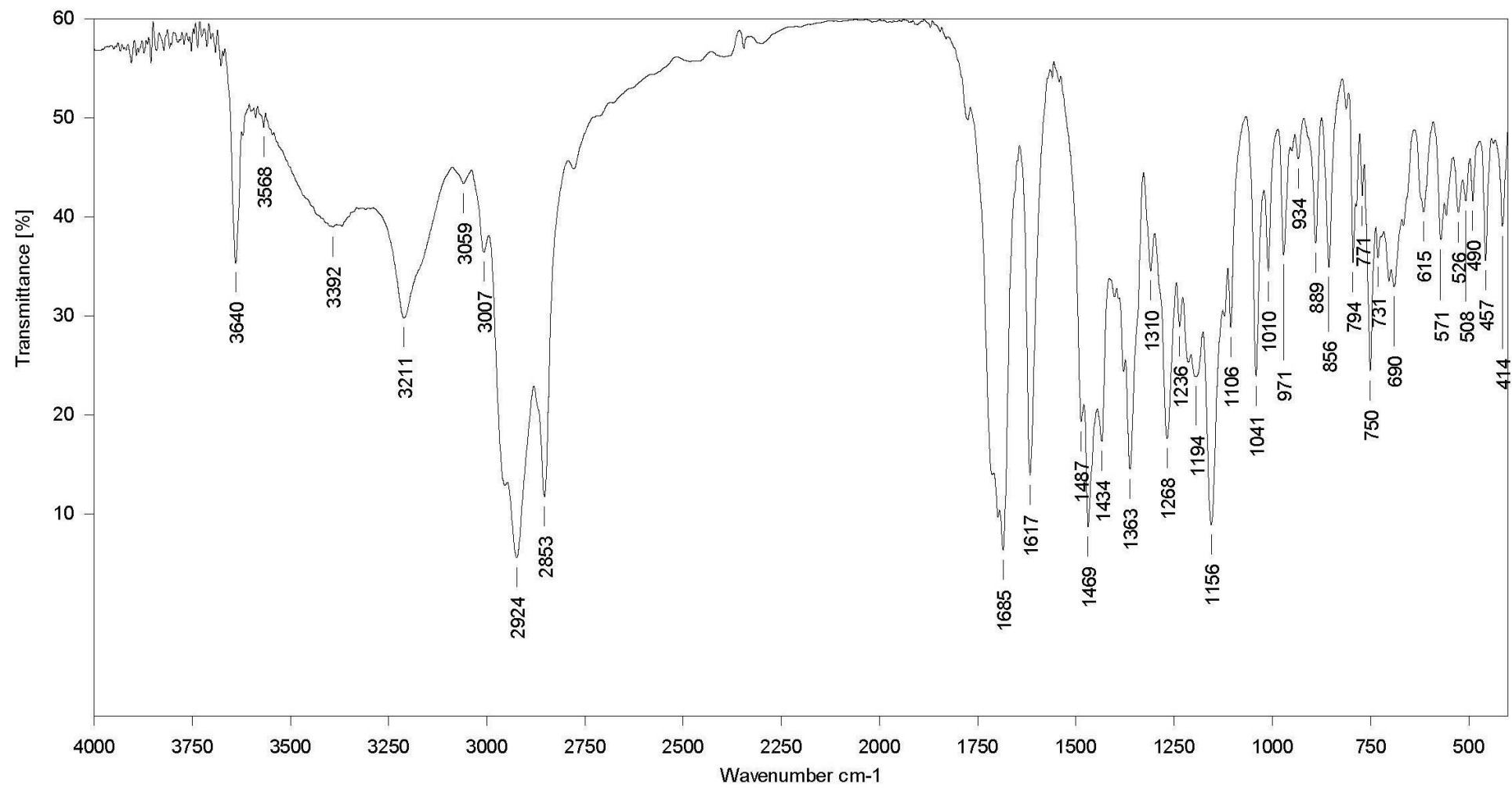


Figure S75. IR spectrum of compound **3c** (in KBr pellet)

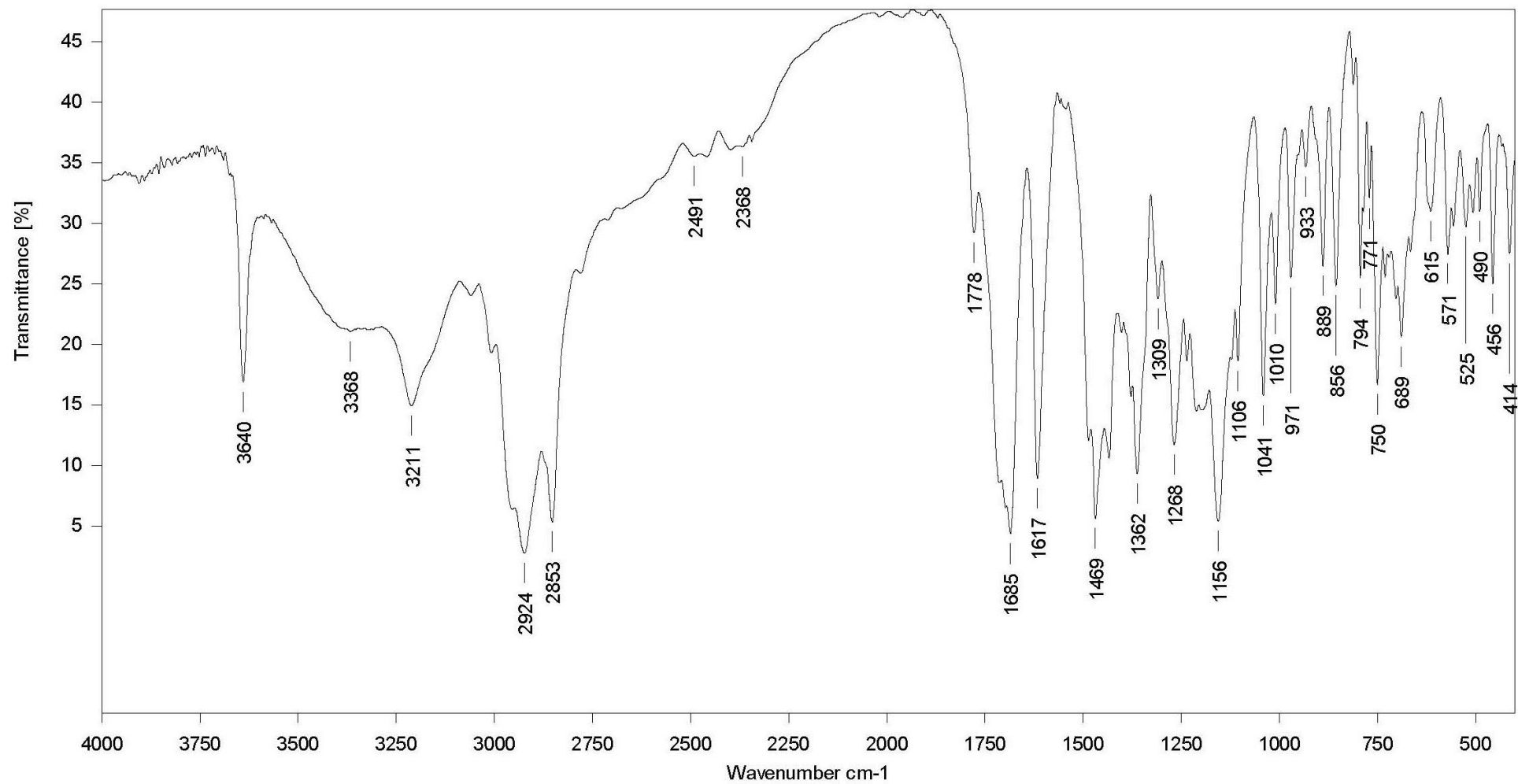


Figure S76. IR spectrum of compound **3d** (in KBr pellet)

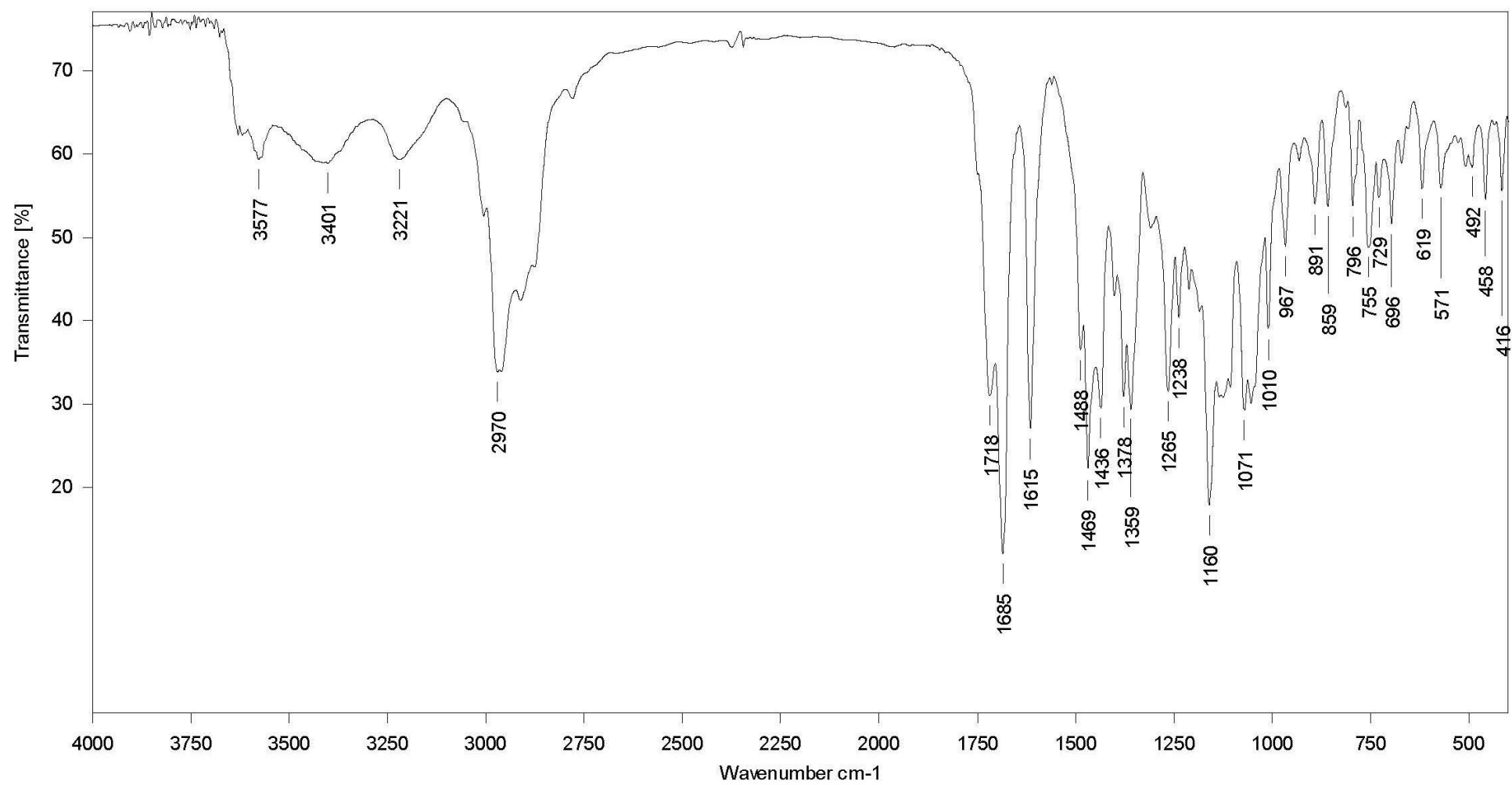


Figure S77. IR spectrum of compound **3e** (in KBr pellet)

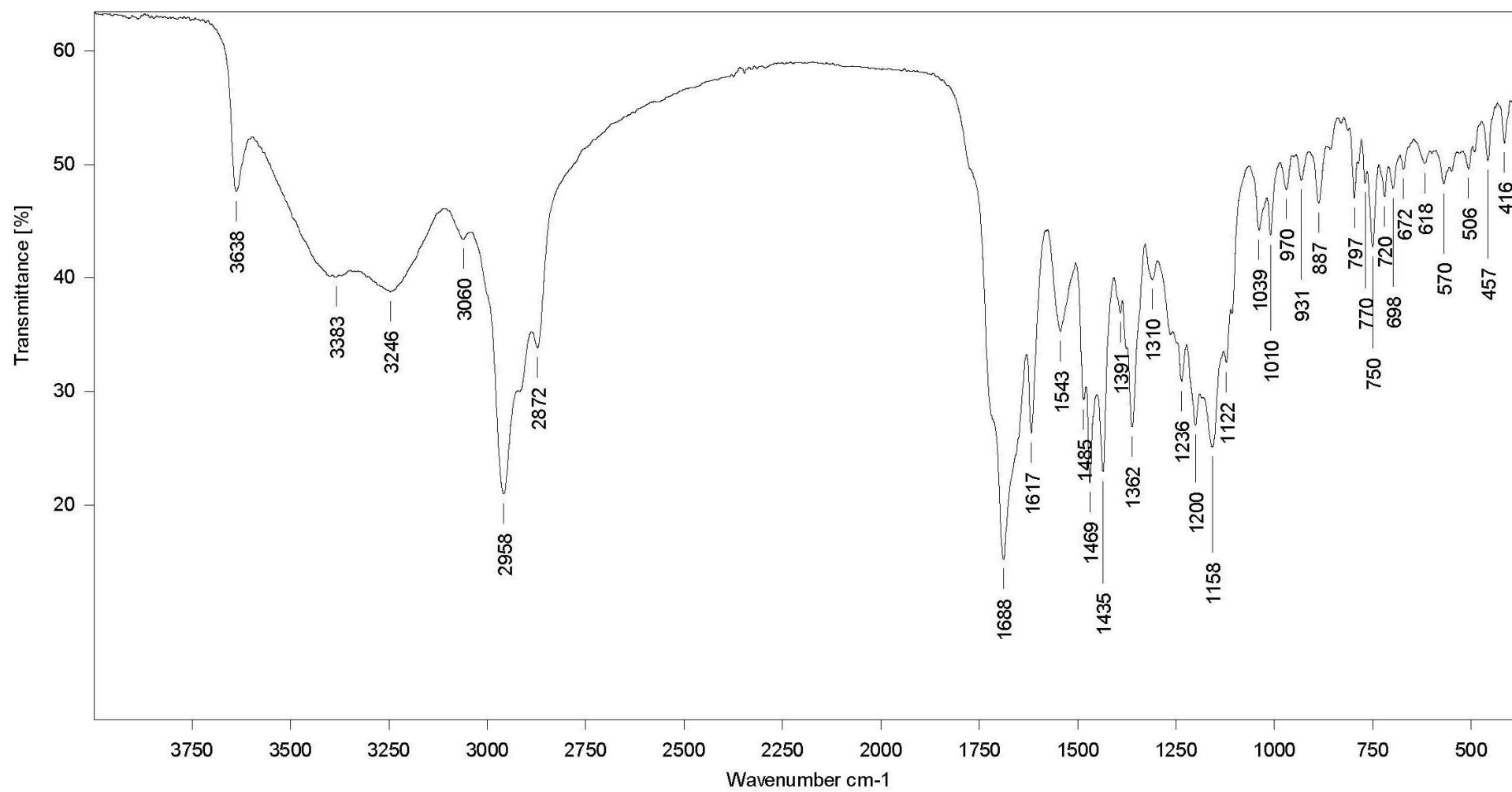


Figure S78. IR spectrum of compound **3f** (in KBr pellet)

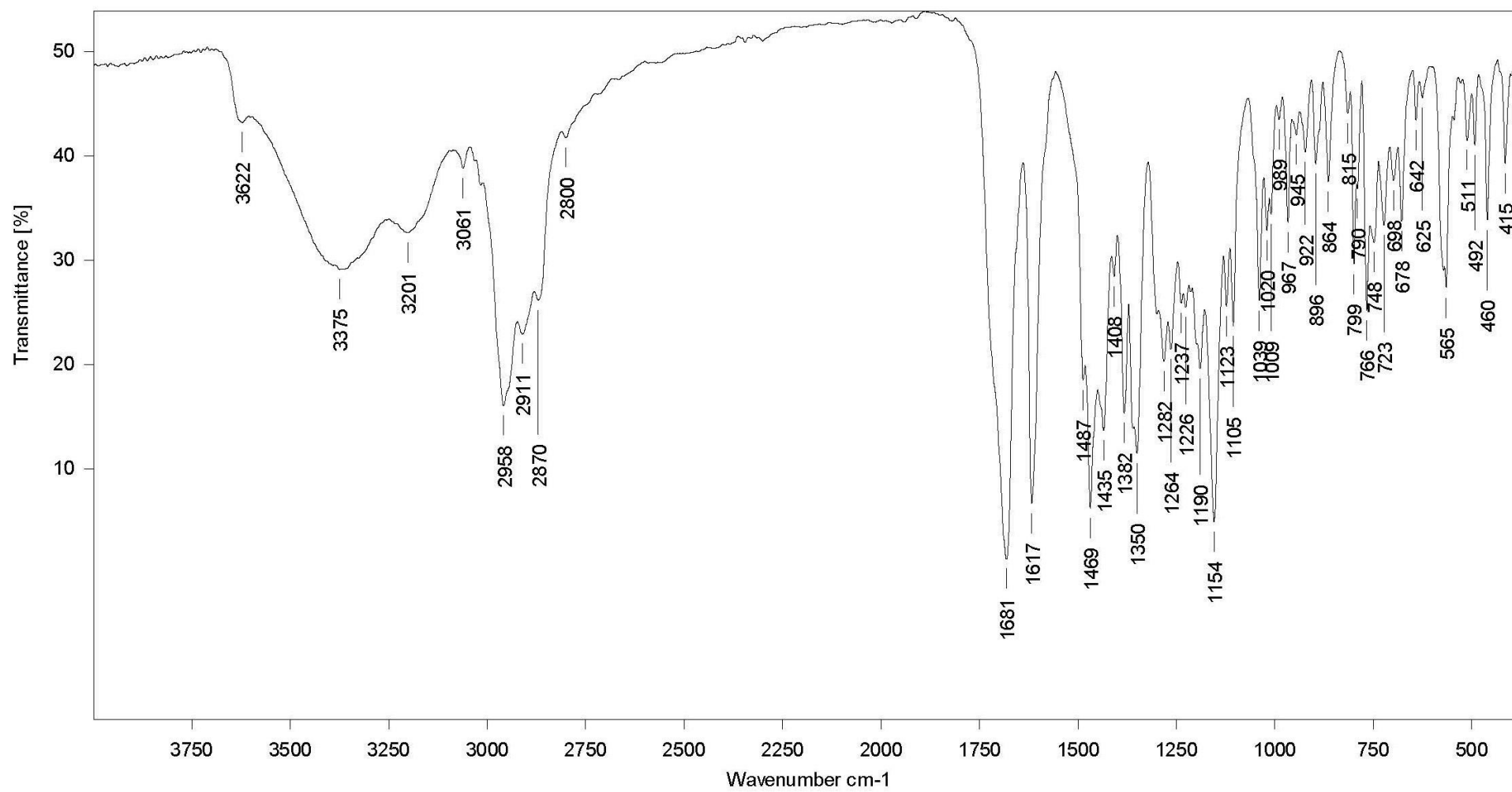


Figure S79. IR spectrum of compound **3g** (in KBr pellet)

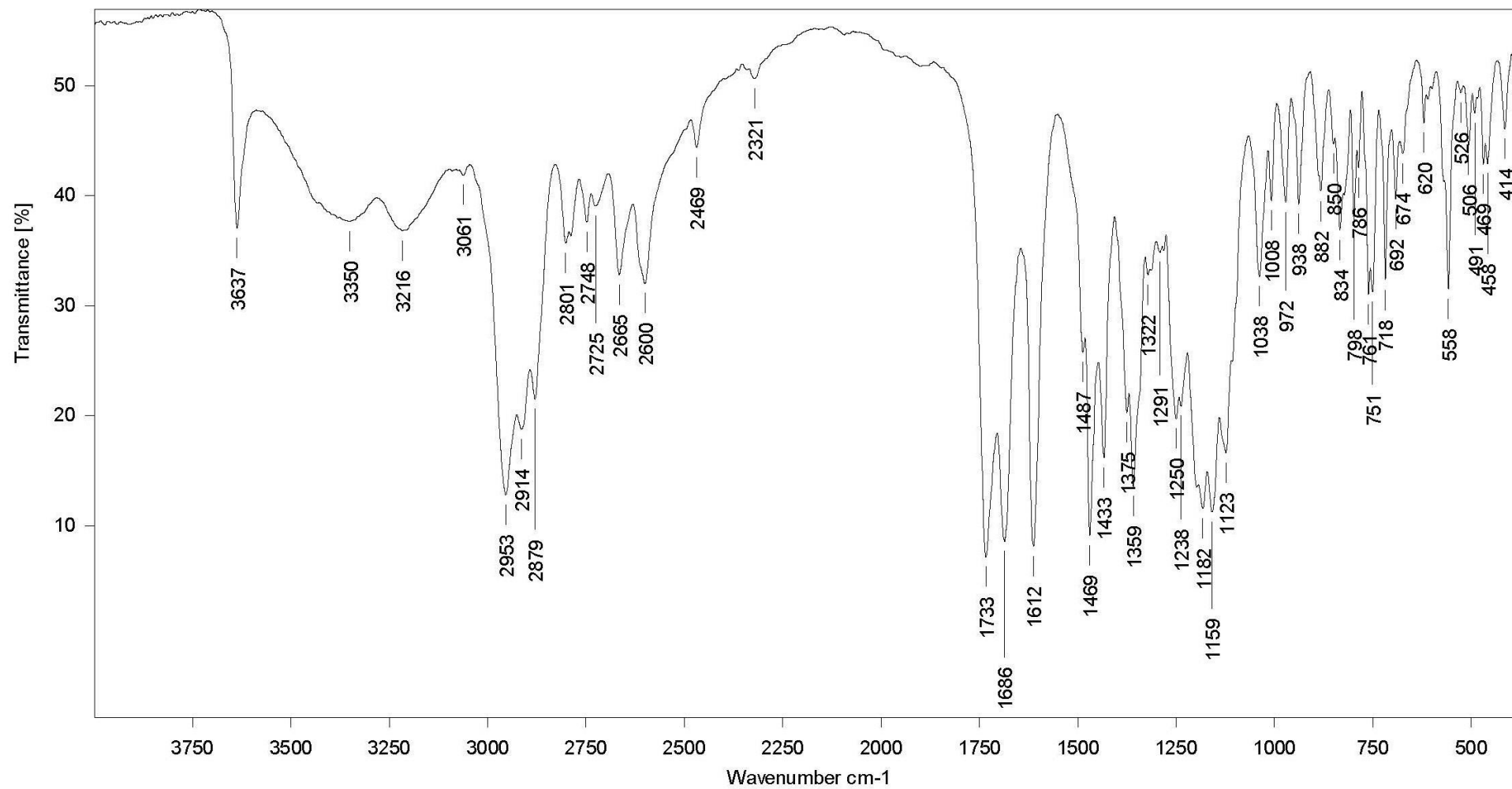


Figure S80. IR spectrum of compound **3h** (in KBr pellet)

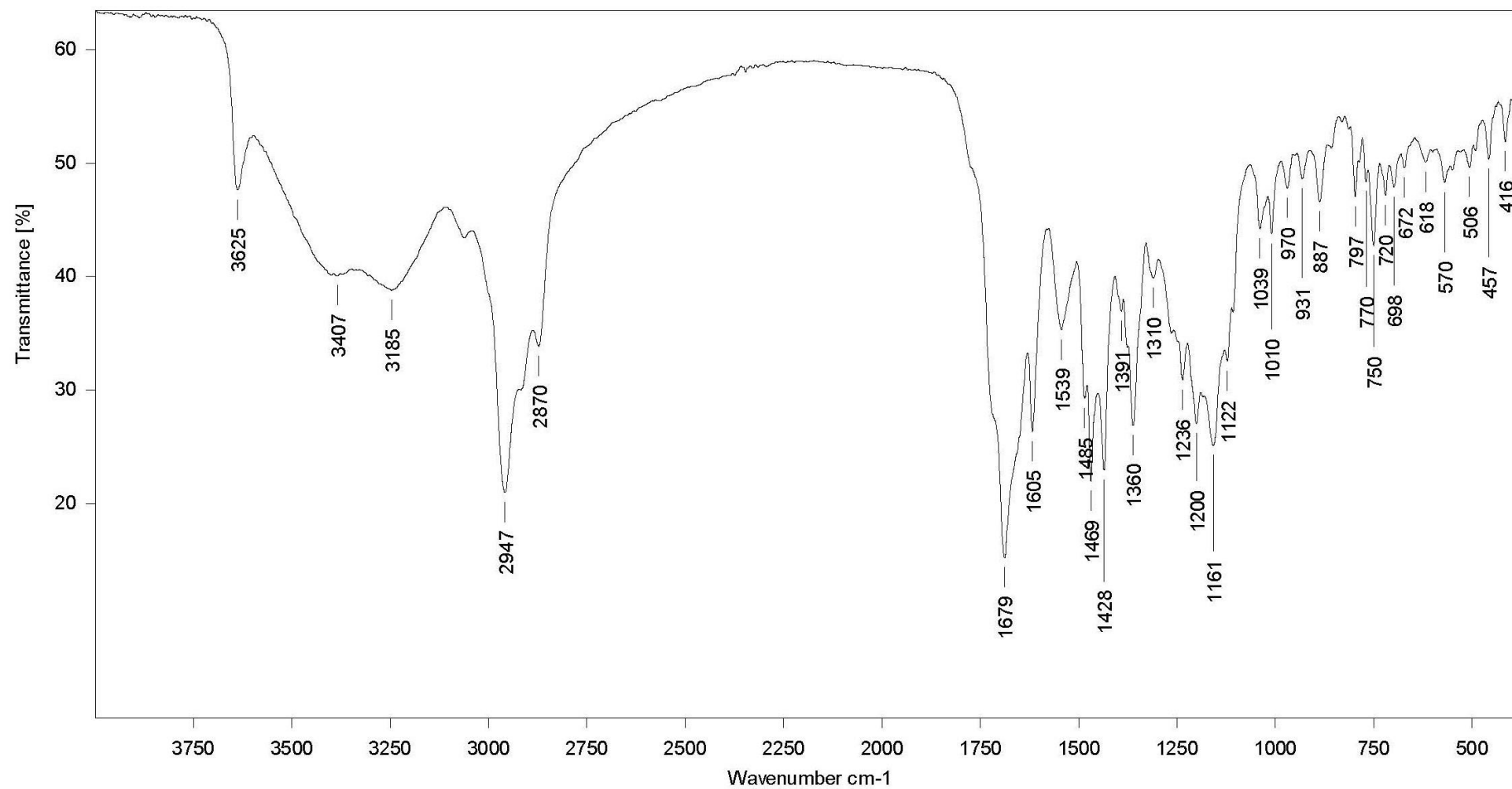


Figure S81. IR spectrum of compound **3i** (in KBr pellet)

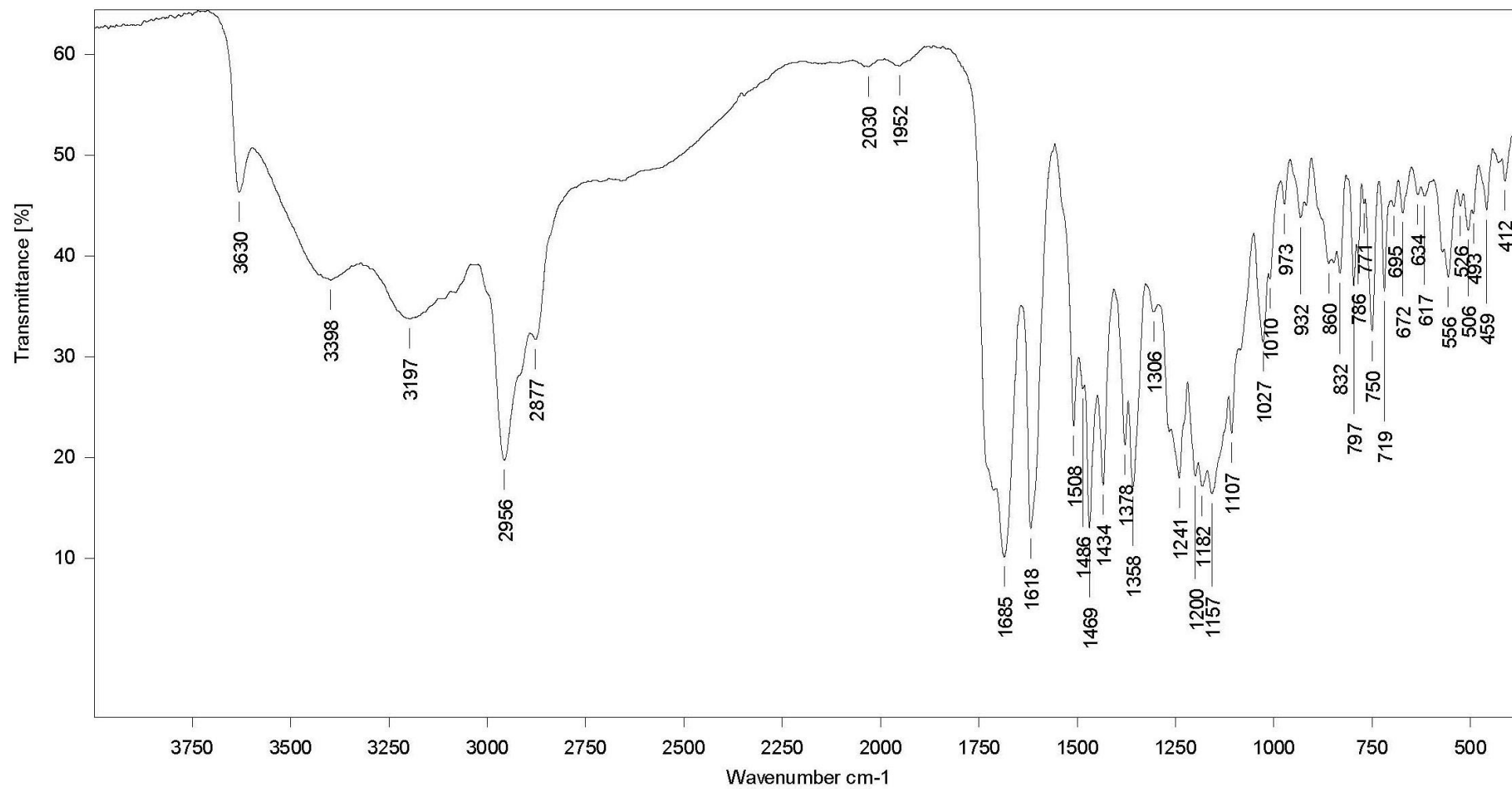


Figure S82. IR spectrum of compound **3j** (in KBr pellet)

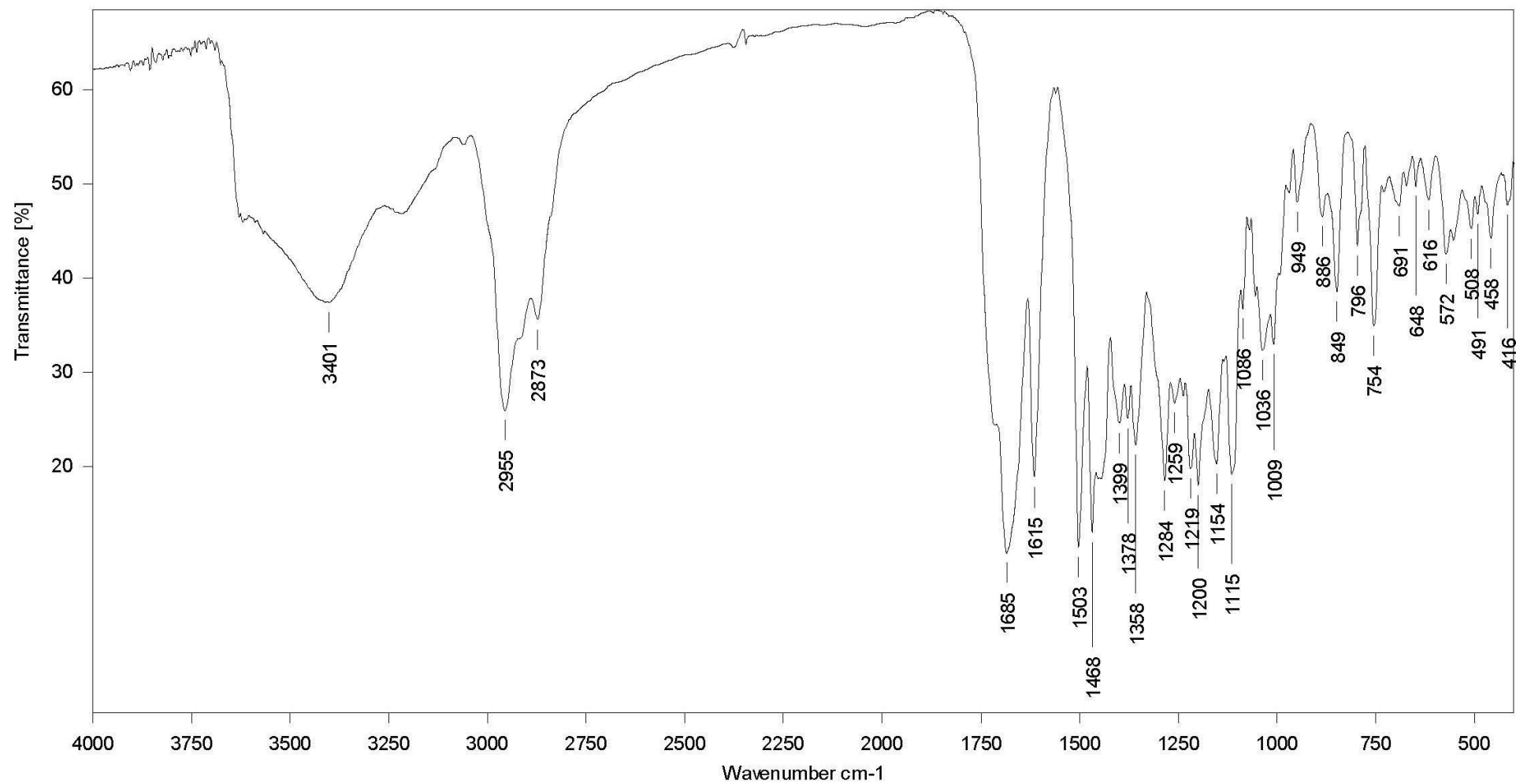


Figure S83. IR spectrum of compound **3k** (in KBr pellet)

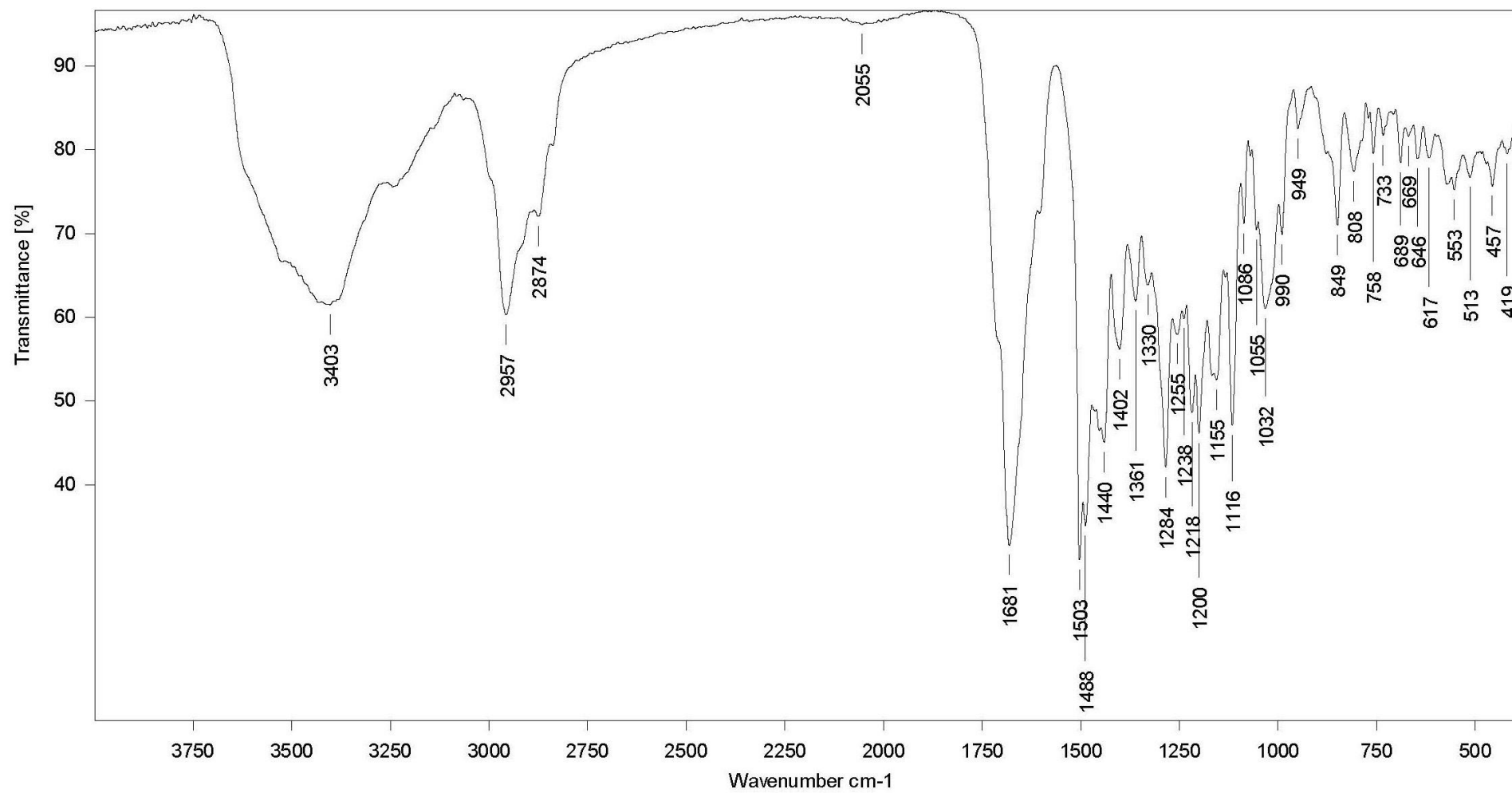


Figure S84. IR spectrum of compound **3I** (in KBr pellet)

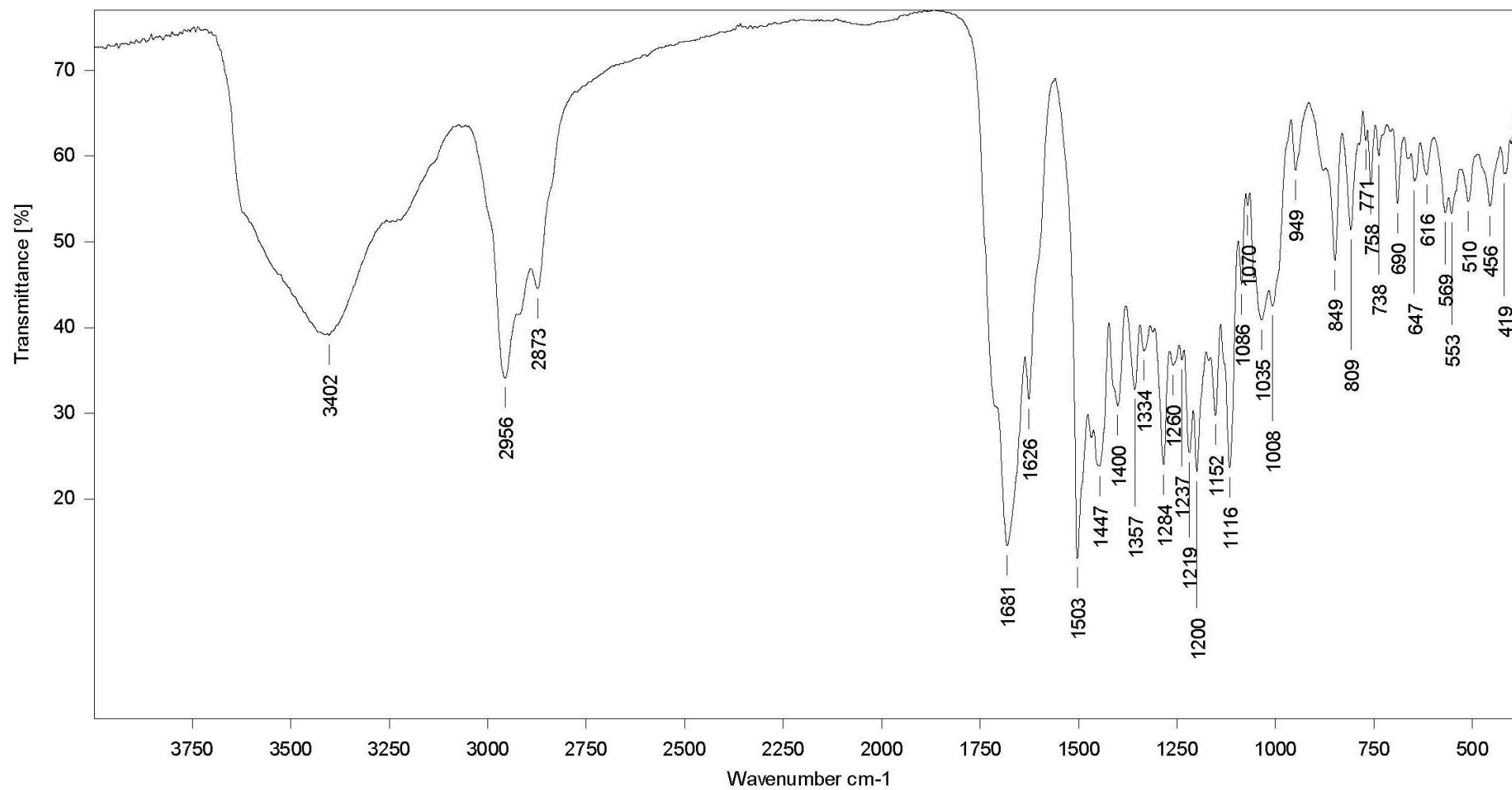


Figure S85. IR spectrum of compound **3m** (in KBr pellet)

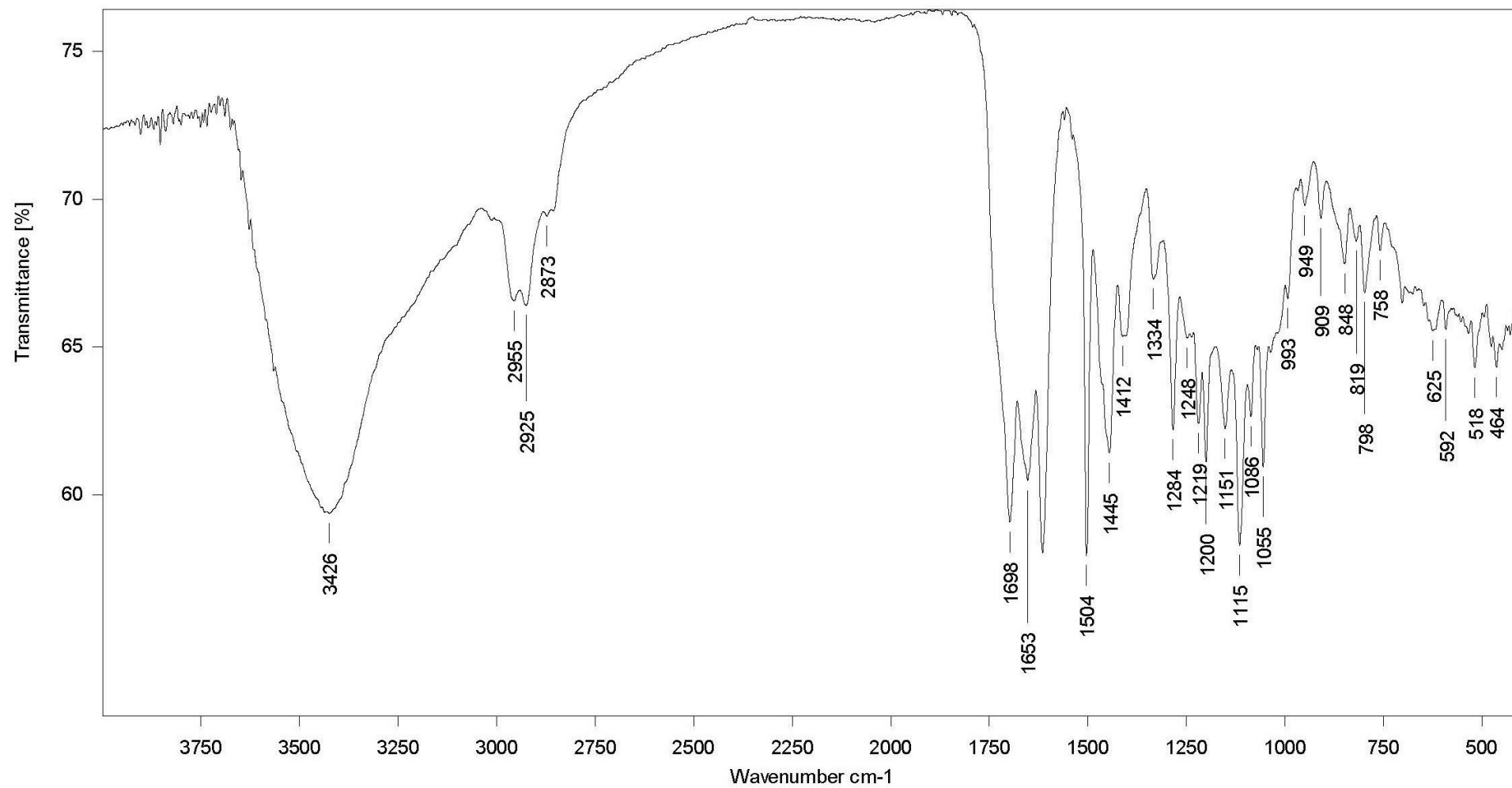
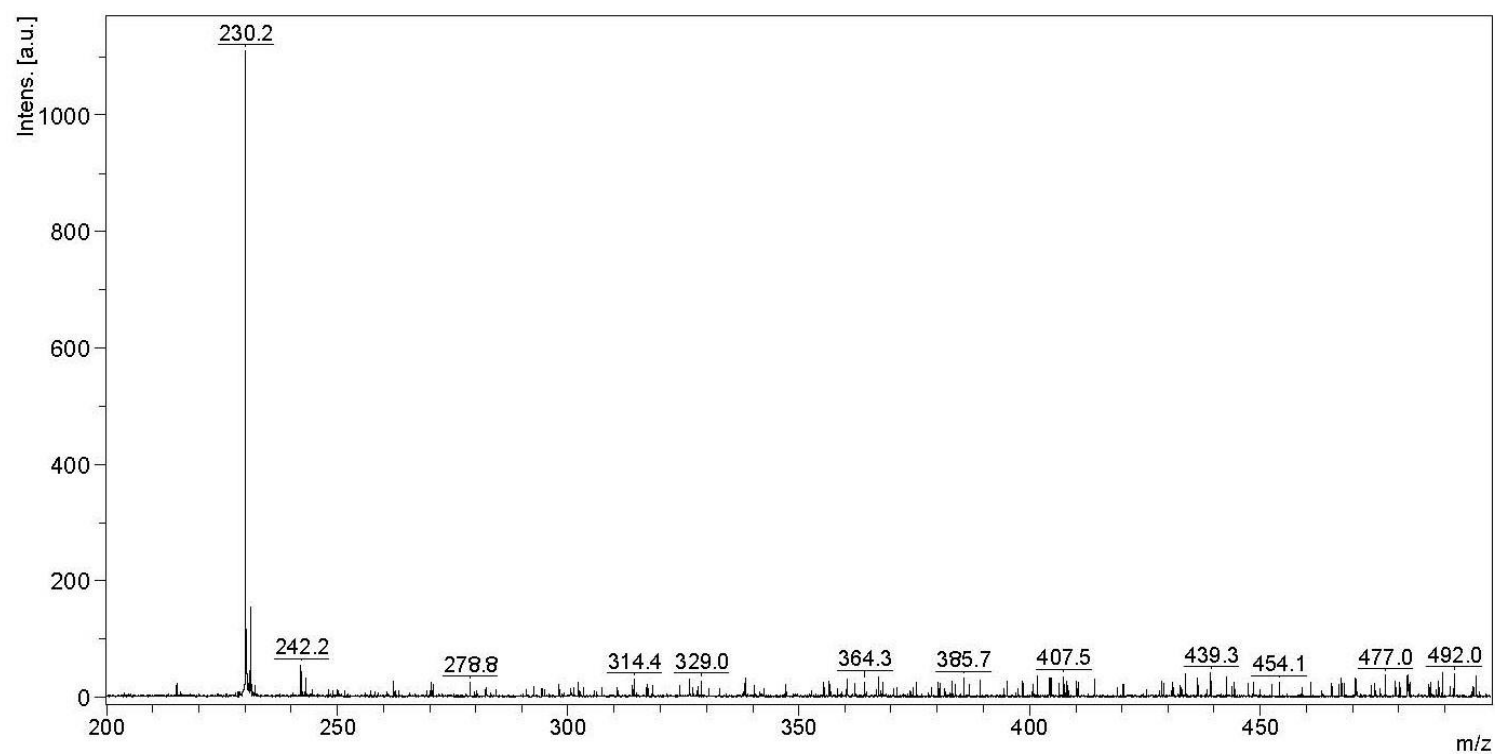


Figure S86. IR spectrum of compound **3n** (in KBr pellet)



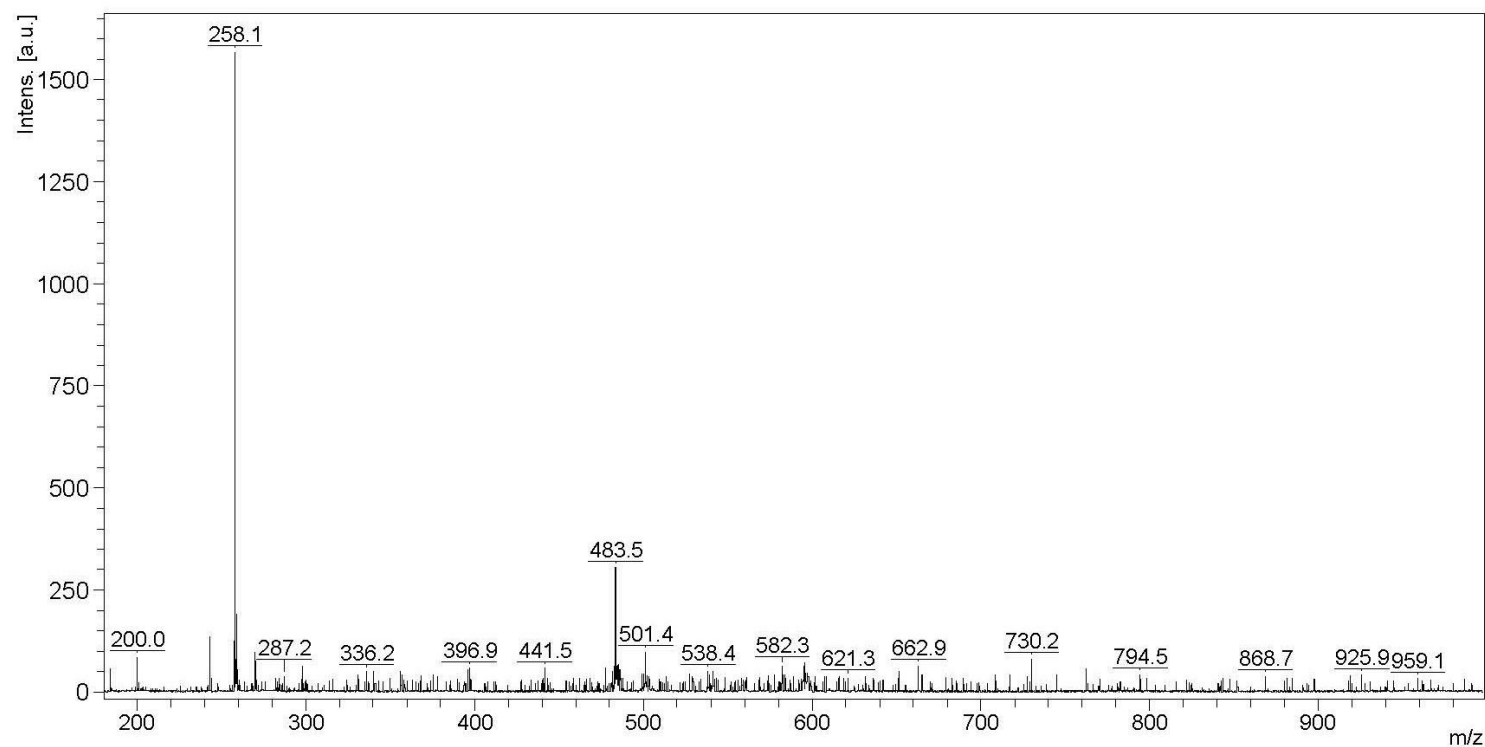
Instrument
 Instrument type: ultraflexTOF/TOF
 Name of computer: MALDI
 flexControl version: flexControl 3.0.173.0
 flexAnalysis version: 3.0.96.0

Spectrometer
 Ion Polarity: POS
 PIE delay: 0 ns
 Ion source voltage 1: 25 kV
 Ion source voltage 2: 23.65 kV
 Lens voltage: 6 kV
 Linear detector voltage: 1.549 kV
 Reflector voltage 1: 0 kV
 Reflector voltage 2: 0 kV
 Reflector detector voltage: 1.569 kV

Laser
 Ion Source Type: MALDI
 Laser Type: Nd:YAG
 Wavelength: 355 nm
 Number of shots: 200
 Laser repetition rate: 100 Hz

Target
 Target Plate: MTP AnchorChip
 Position: L8

Figure S87. MALDI spectrum of compound **1a**



Instrument

Instrument type	ultraflexTOF/TOF
Name of computer	MALDI
flexControl version	flexControl 3.0.173.0
flexAnalysis version	3.0.96.0

Spectrometer

Ion Polarity	POS
PIE delay	0 ns
Ion source voltage 1	25 kV
Ion source voltage 2	23.65 kV
Lens voltage	6 kV
Linear detector voltage	1.549 kV
Reflector voltage 1	0 kV
Reflector voltage 2	0 kV
Reflector detector voltage	1.569 kV

Laser

Ion Source Type	MALDI
Laser Type	Nd:YAG
Wavelength	355 nm
Number of shots	200
Laser repetition rate	100 Hz

Target

Target Plate	MTP AnchorChip
Position	E2

Figure S88. MALDI spectrum of compound **1b**

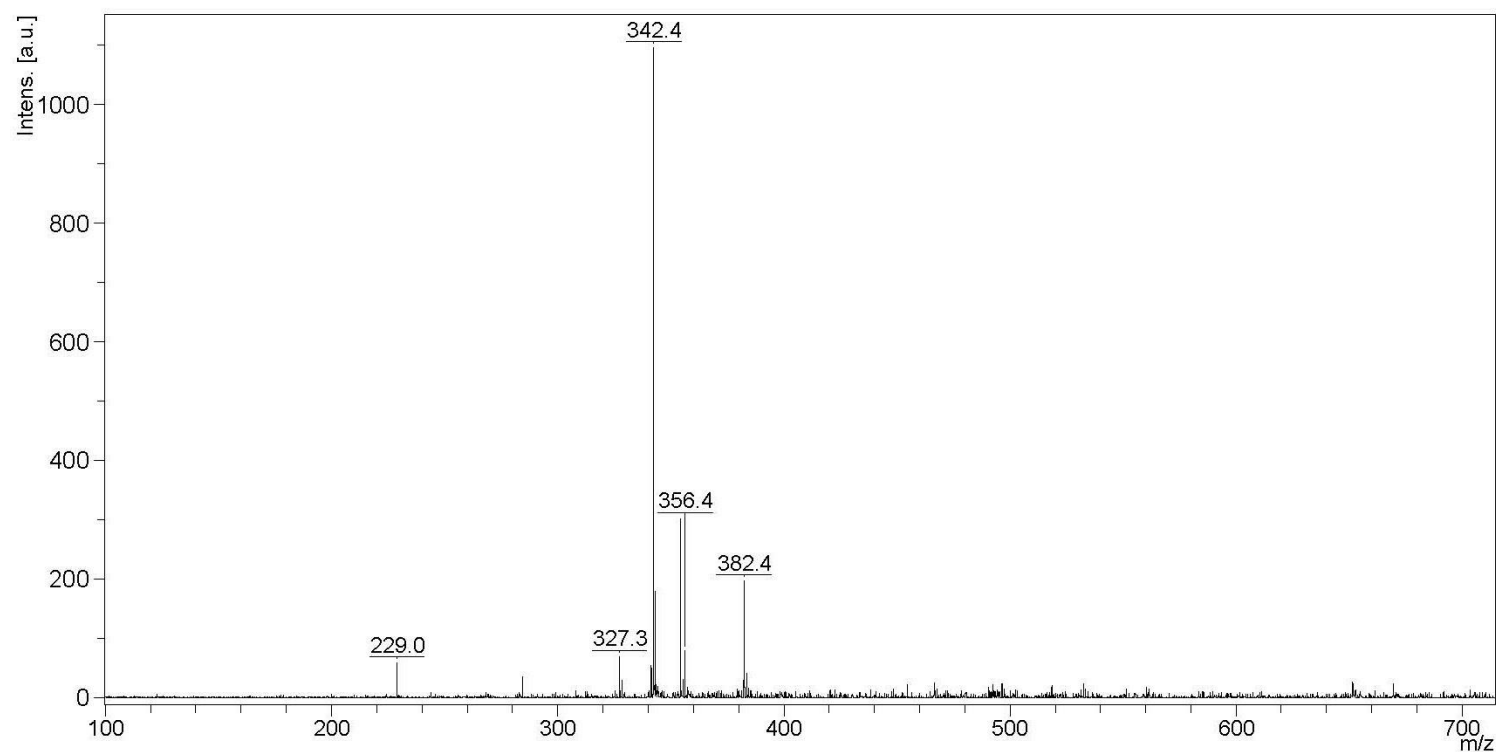


Figure S89. MALDI spectrum of compound **1c**

Instrument

Instrument type	ultraflexTOF/TOF
Name of computer	MALDI
flexControl version	flexControl 3.0.173.0
flexAnalysis version	3.0.96.0

Spectrometer

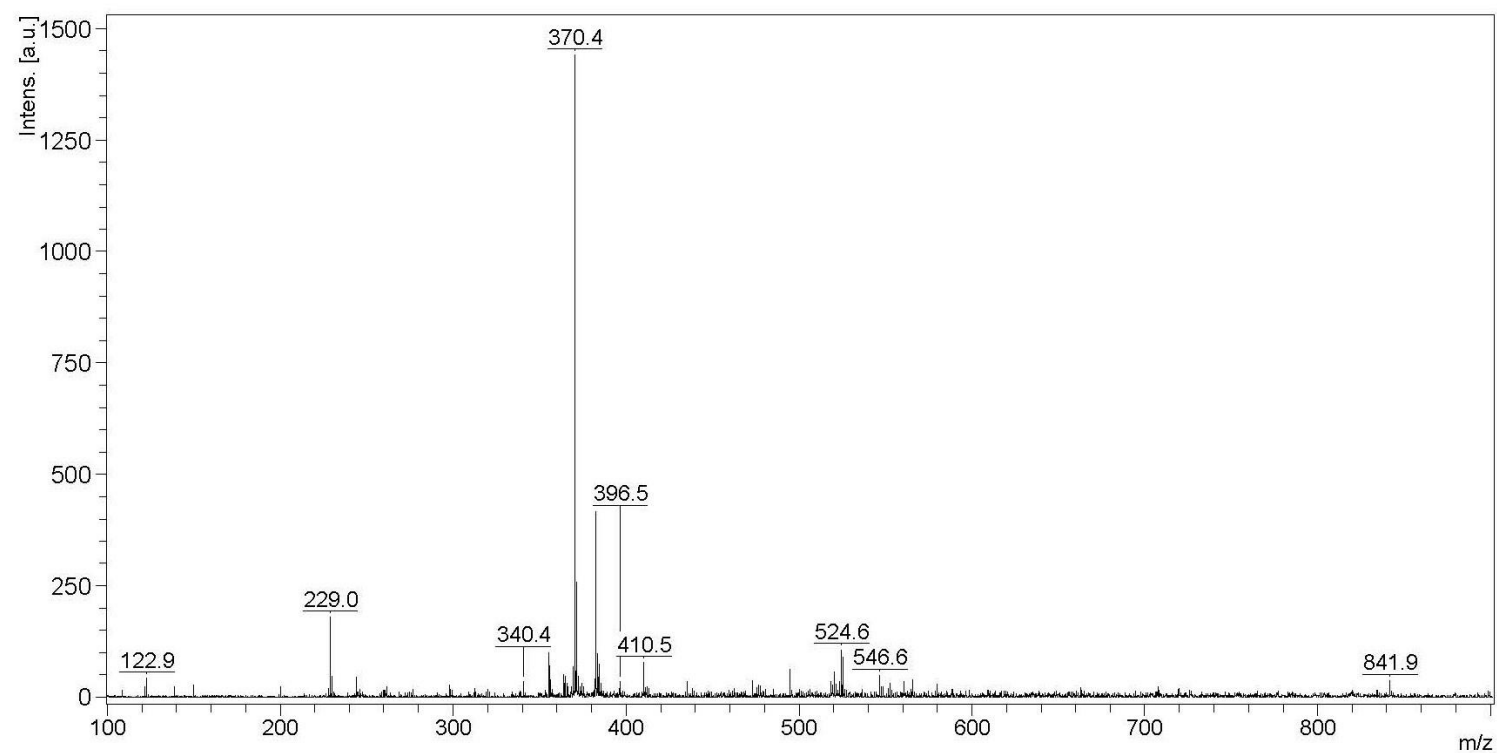
Ion Polarity	POS
PIE delay	30 ns
Ion source voltage 1	20 kV
Ion source voltage 2	19.01 kV
Lens voltage	5 kV
Linear detector voltage	1.44 kV
Reflector voltage 1	0 kV
Reflector voltage 2	0 kV
Reflector detector voltage	1.569 kV

Laser

Ion Source Type	MALDI
Laser Type	Nd:YAG
Wavelength	355 nm
Number of shots	50
Laser repetition rate	100 Hz

Target

Target Plate	MTP AnchorChip
Position	N14



Instrument

Instrument type: ultraflexTOF/TOF
 Name of computer: MALDI
 flexControl version: flexControl 3.0.173.0
 flexAnalysis version: 3.0.96.0

Spectrometer

Ion Polarity: POS
 PIE delay: 30 ns
 Ion source voltage 1: 20 kV
 Ion source voltage 2: 19.01 kV
 Lens voltage: 5 kV
 Linear detector voltage: 1.44 kV
 Reflector voltage 1: 0 kV
 Reflector voltage 2: 0 kV
 Reflector detector voltage: 1.569 kV

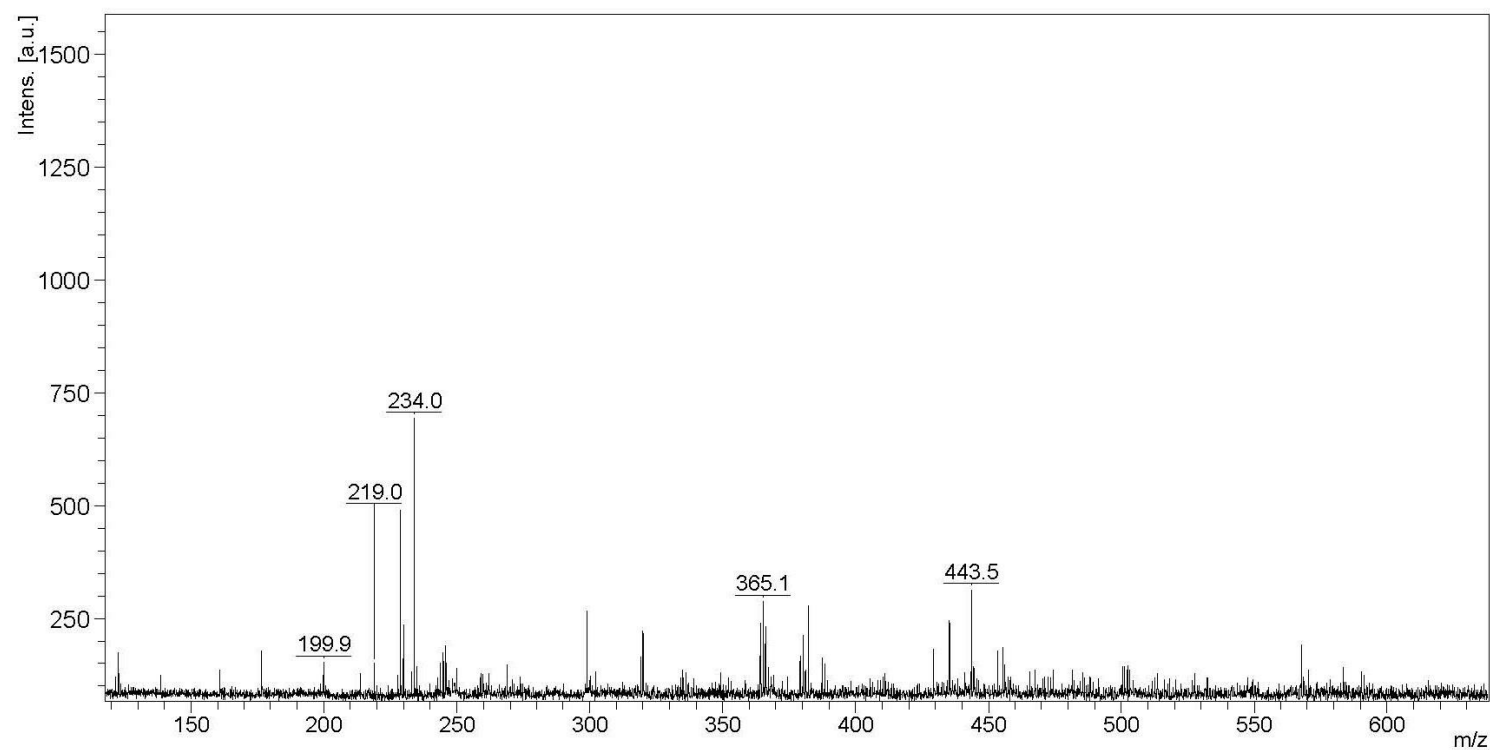
Laser

Ion Source Type: MALDI
 Laser Type: Nd:YAG
 Wavelength: 355 nm
 Number of shots: 150
 Laser repetition rate: 100 Hz

Target

Target Plate: MTP AnchorChip
 Position: N15

Figure S90. MALDI spectrum of compound **1d**



Instrument

Instrument type: ultraflexTOF/TOF
 Name of computer: MALDI
 flexControl version: flexControl 3.0.173.0
 flexAnalysis version: 3.0.96.0

Spectrometer

Ion Polarity: POS
 PIE delay: 50 ns
 Ion source voltage 1: 20 kV
 Ion source voltage 2: 19.01 kV
 Lens voltage: 6 kV
 Linear detector voltage: 1.498 kV
 Reflector voltage 1: 0 kV
 Reflector voltage 2: 0 kV
 Reflector detector voltage: 1.497 kV

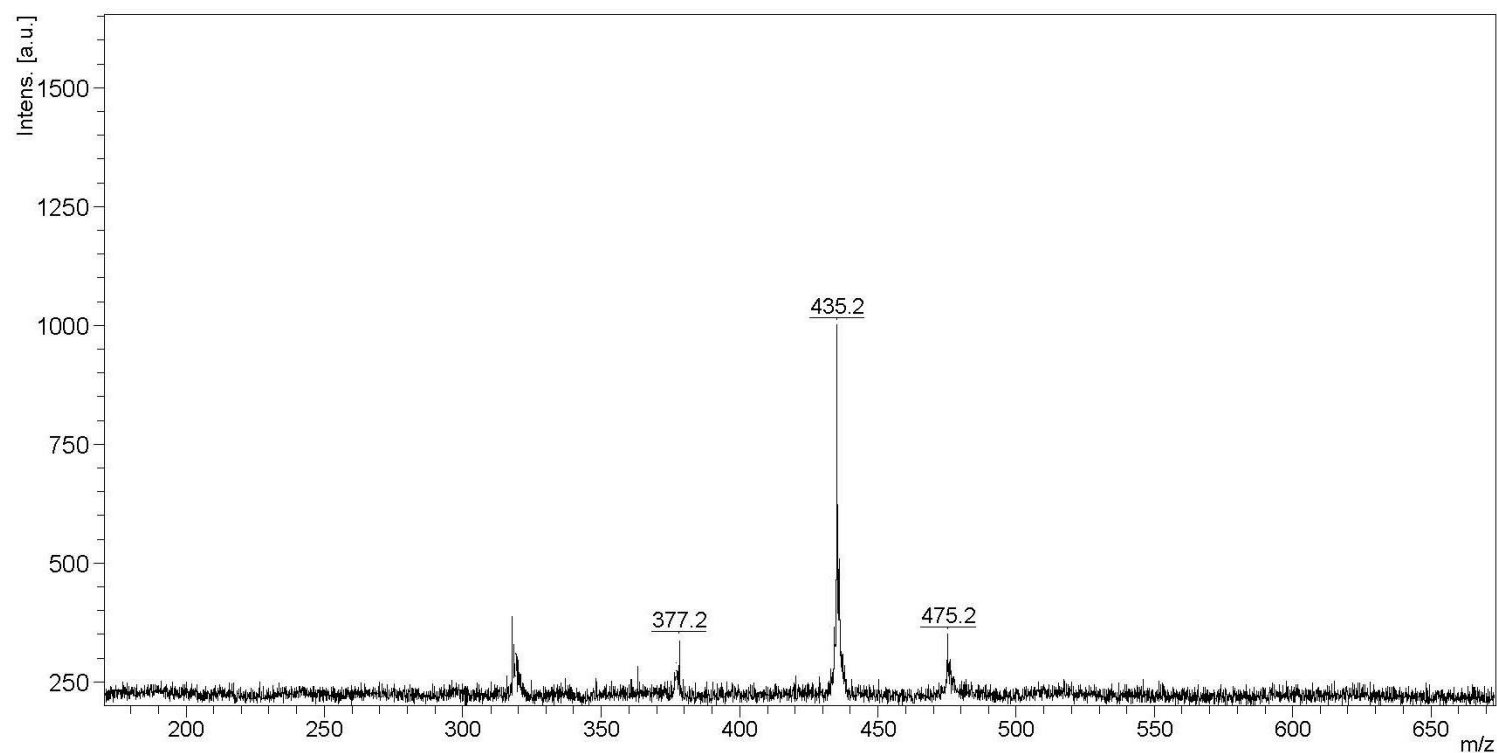
Laser

Ion Source Type: MALDI
 Laser Type: Nd:YAG
 Wavelength: 355 nm
 Number of shots: 100
 Laser repetition rate: 100 Hz

Target

Target Plate: MTP AnchorChip
 Position: F11

Figure S91. MALDI spectrum of compound **1e**



Instrument

Instrument type	ultraflexTOF/TOF
Name of computer	MALDI
flexControl version	flexControl 3.0.173.0
flexAnalysis version	3.0.96.0

Spectrometer

Ion Polarity	POS
PIE delay	50 ns
Ion source voltage 1	20 kV
Ion source voltage 2	19.01 kV
Lens voltage	6 kV
Linear detector voltage	1.498 kV
Reflector voltage 1	0 kV
Reflector voltage 2	0 kV
Reflector detector voltage	1.497 kV

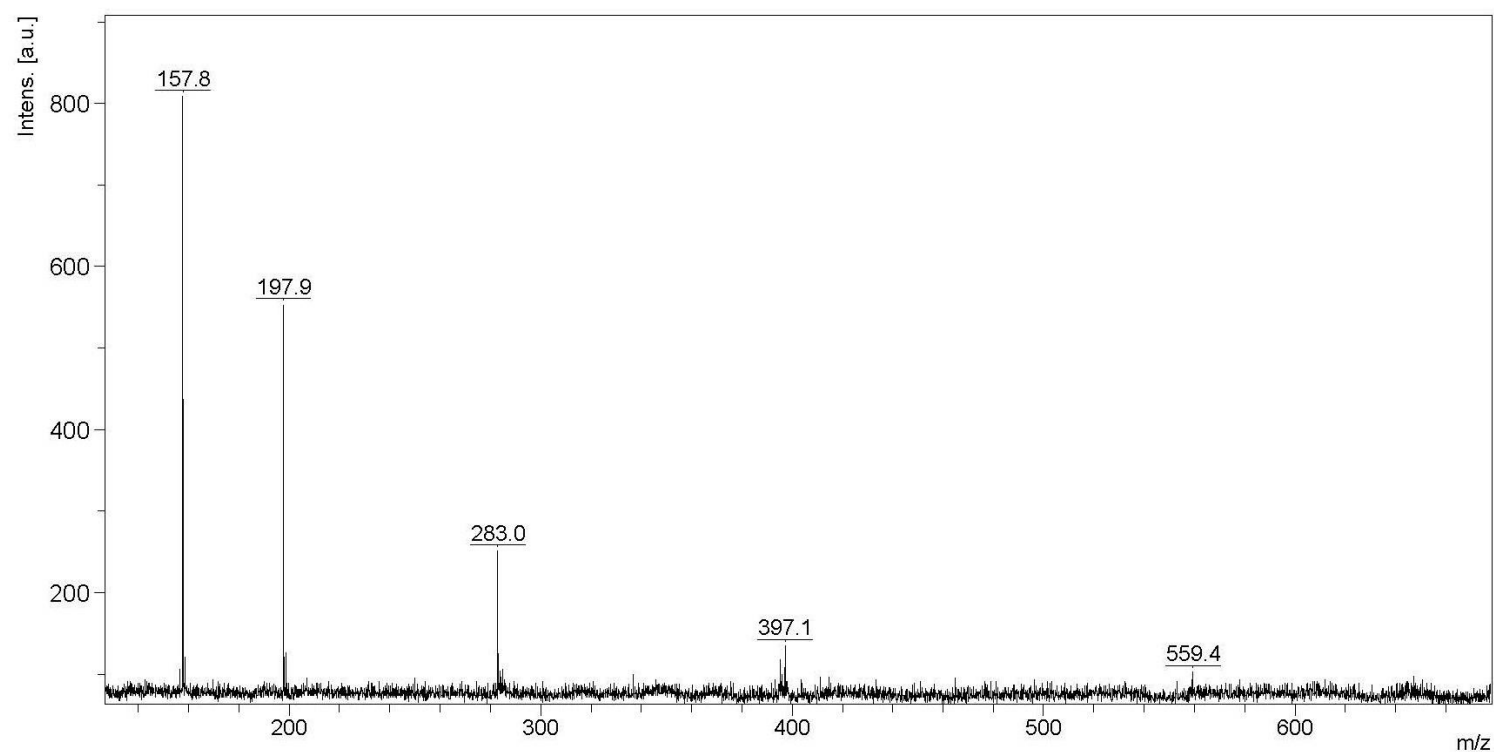
Laser

Ion Source Type	MALDI
Laser Type	Nd:YAG
Wavelength	355 nm
Number of shots	300
Laser repetition rate	100 Hz

Target

Target Plate	MTP AnchorChip
Position	N6

Figure S92. MALDI spectrum of compound **1f**



Instrument

Instrument type	ultraflexTOF/TOF
Name of computer	MALDI
flexControl version	flexControl 3.0.173.0
flexAnalysis version	3.0.96.0

Spectrometer

Ion Polarity	POS
PIE delay	50 ns
Ion source voltage 1	20 kV
Ion source voltage 2	19.01 kV
Lens voltage	6 kV
Linear detector voltage	1.498 kV
Reflector voltage 1	0 kV
Reflector voltage 2	0 kV
Reflector detector voltage	1.497 kV

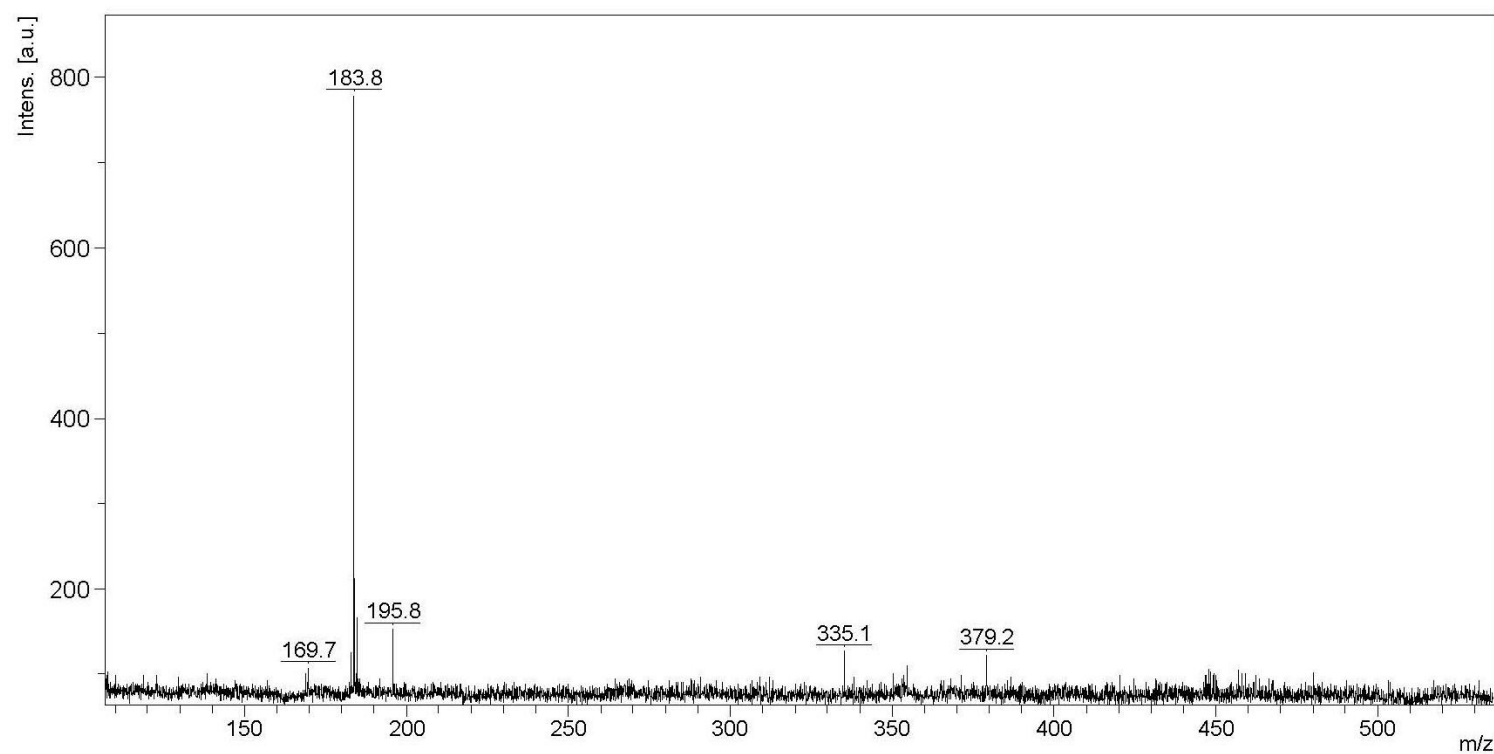
Laser

Ion Source Type	MALDI
Laser Type	Nd:YAG
Wavelength	355 nm
Number of shots	100
Laser repetition rate	100 Hz

Target

Target Plate	MTP AnchorChip
Position	M20

Figure S93. MALDI spectrum of compound **1g**



Instrument

Instrument type: ultraflexTOF/TOF
Name of computer: MALDI
flexControl version: flexControl 3.0.173.0
flexAnalysis version: 3.0.96.0

Spectrometer

Ion Polarity: POS
PIE delay: 50 ns
Ion source voltage 1: 20 kV
Ion source voltage 2: 19.01 kV
Lens voltage: 6 kV
Linear detector voltage: 1.498 kV
Reflector voltage 1: 0 kV
Reflector voltage 2: 0 kV
Reflector detector voltage: 1.497 kV

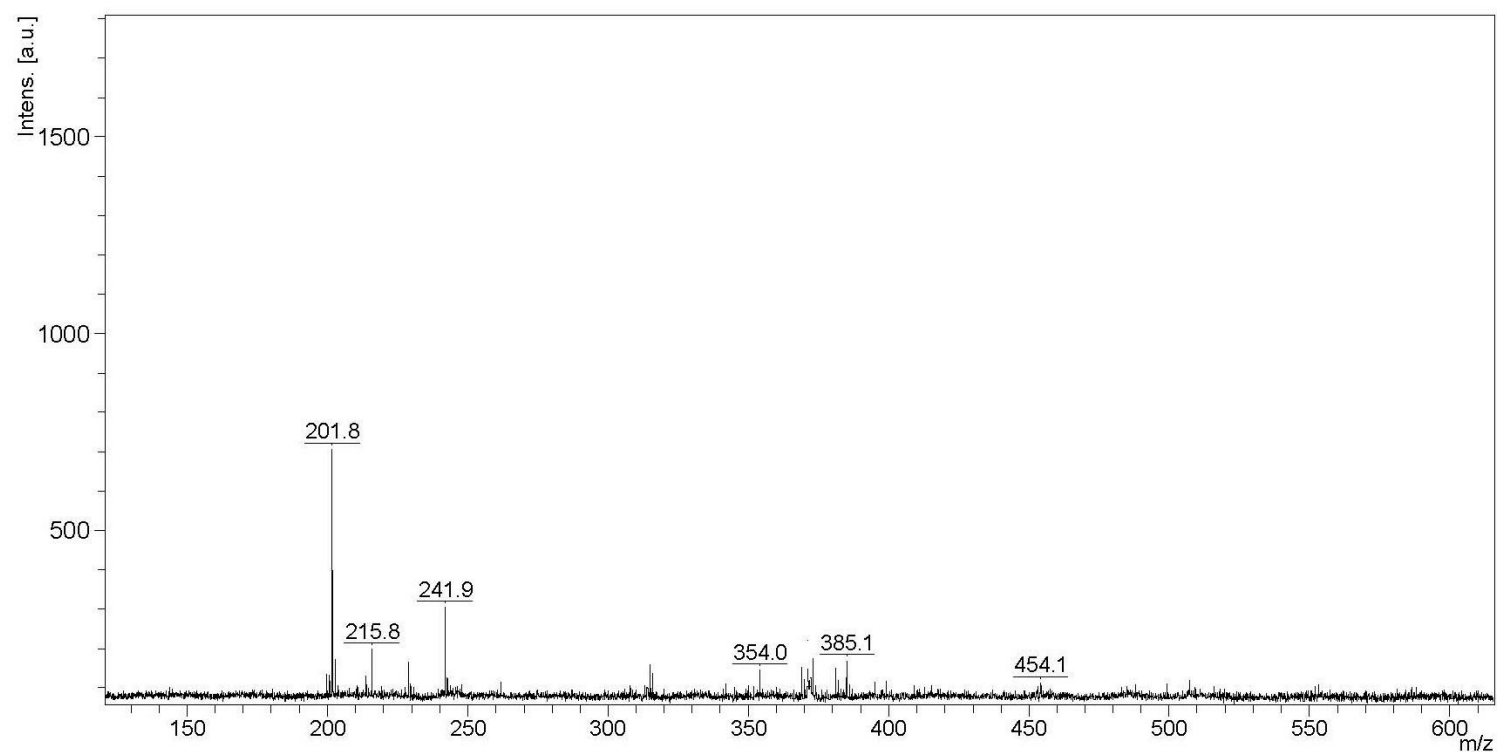
Laser

Ion Source Type: MALDI
Laser Type: Nd:YAG
Wavelength: 355 nm
Number of shots: 100
Laser repetition rate: 100 Hz

Target

Target Plate: MTP AnchorChip
Position: G9

Figure S94. MALDI spectrum of compound **1h**



Instrument

Instrument type	ultraflexTOF/TOF
Name of computer	MALDI
flexControl version	flexControl 3.0.173.0
flexAnalysis version	3.0.96.0

Spectrometer

Ion Polarity	POS
PIE delay	50 ns
Ion source voltage 1	20 kV
Ion source voltage 2	19.01 kV
Lens voltage	6 kV
Linear detector voltage	1.498 kV
Reflector voltage 1	0 kV
Reflector voltage 2	0 kV
Reflector detector voltage	1.497 kV

Laser

Ion Source Type	MALDI
Laser Type	Nd:YAG
Wavelength	355 nm
Number of shots	100
Laser repetition rate	100 Hz

Target

Target Plate	MTP AnchorChip
Position	N8

Figure S95. MALDI spectrum of compound **1i**

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	70 m/z	Scan End	3000 m/z
Capillary Exit	140.0 V	n/a	n/a	Trap Drive	54.3
Accumulation Time	590 μ s	Averages	5 Spectra	n/a	n/a

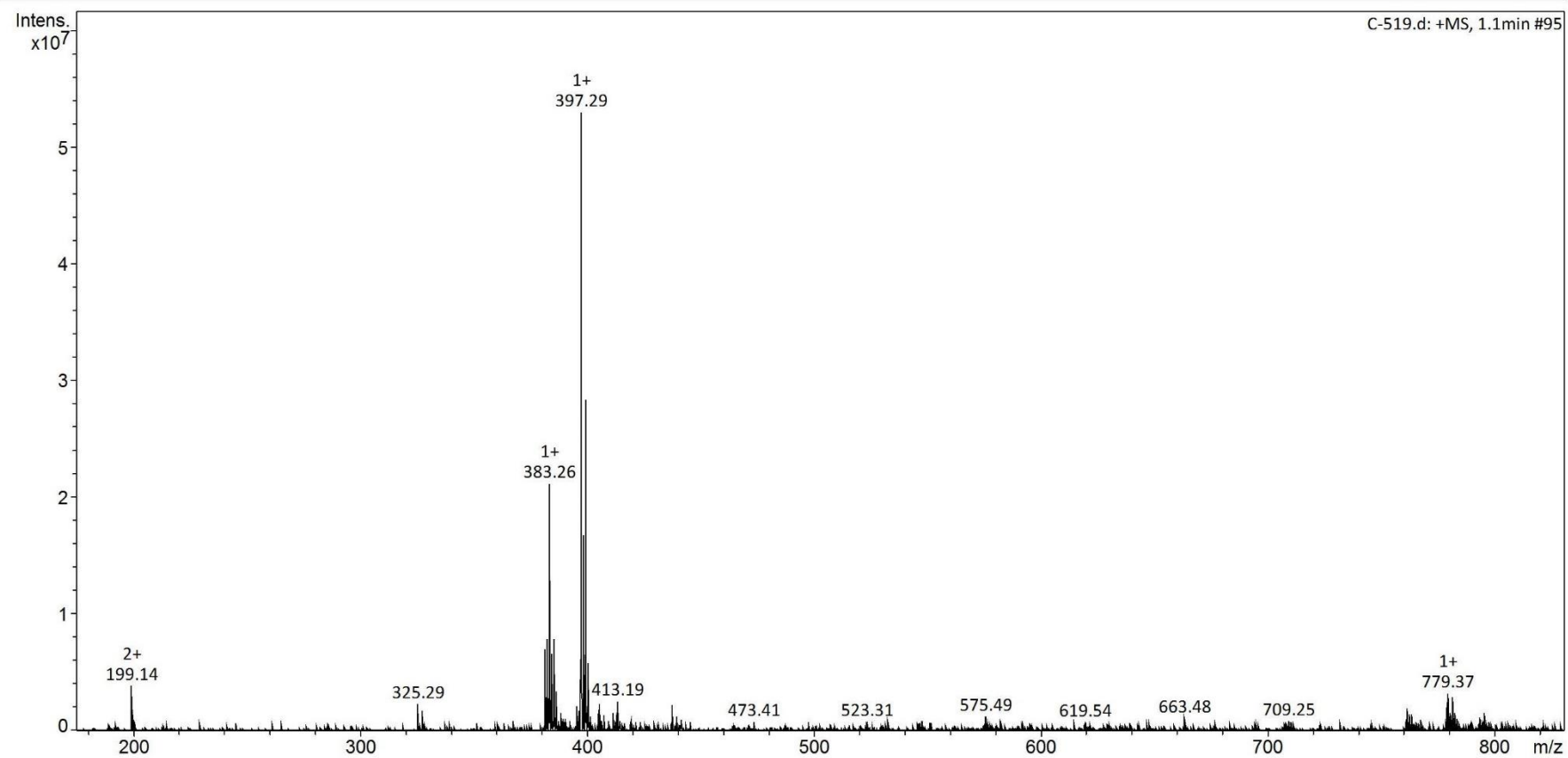


Figure S96. ESI spectrum of compound **1j**

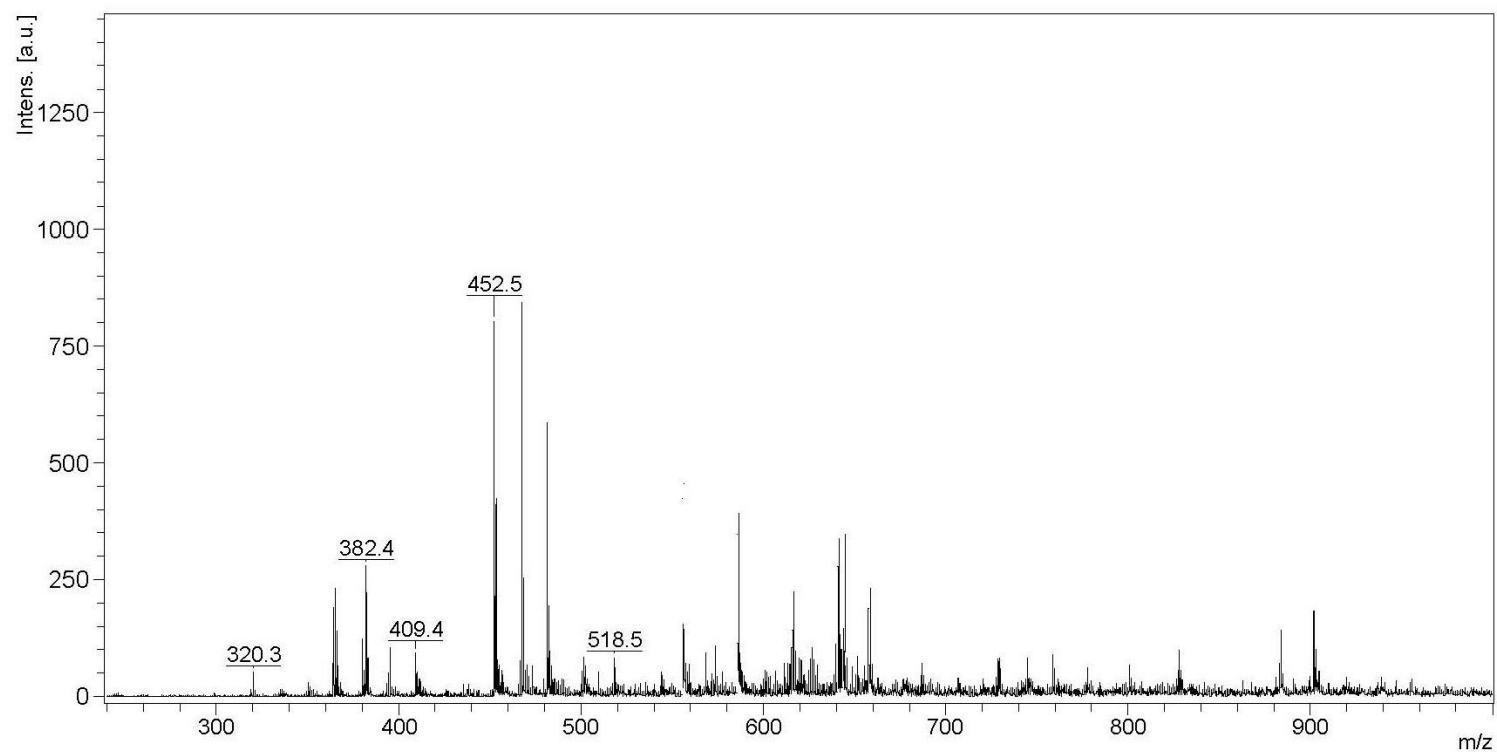


Figure S97. MALDI spectrum of compound **1k**

Instrument

Instrument type	ultraflexTOF/TOF
Name of computer	MALDI
flexControl version	flexControl 3.0.173.0
flexAnalysis version	3.0.96.0

Spectrometer

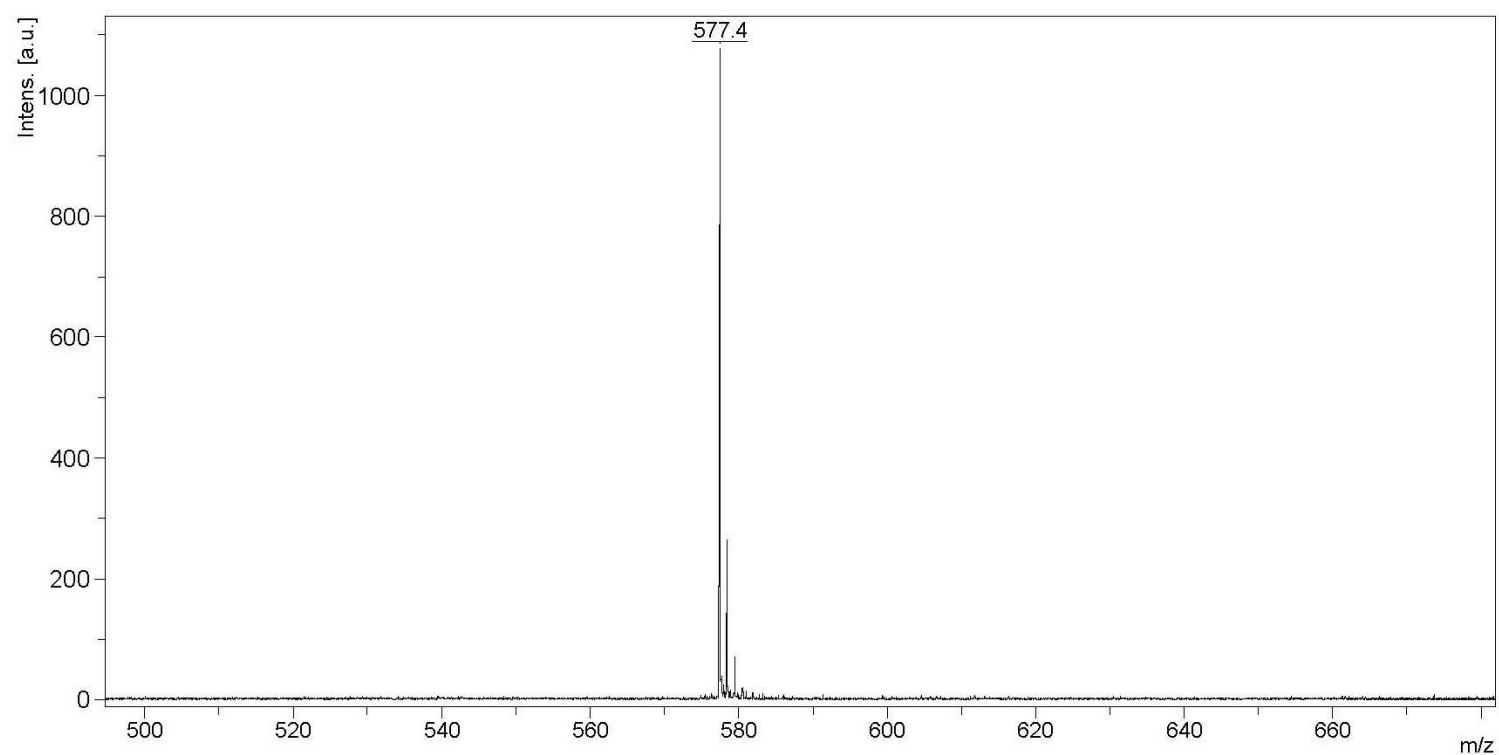
Ion Polarity	POS
PIE delay	50 ns
Ion source voltage 1	20 kV
Ion source voltage 2	19.01 kV
Lens voltage	5 kV
Linear detector voltage	1.44 kV
Reflector voltage 1	0 kV
Reflector voltage 2	0 kV
Reflector detector voltage	0 kV

Laser

Ion Source Type	MALDI
Laser Type	Nd:YAG
Wavelength	355 nm
Number of shots	50
Laser repetition rate	100 Hz

Target

Target Plate	MTP AnchorChip
Position	J3

**Instrument**

Instrument type	ultraflexTOF/TOF
Name of computer	MALDI
flexControl version	flexControl 3.0.173.0
flexAnalysis version	3.0.96.0

Spectrometer

Ion Polarity	POS
PIE delay	30 ns
Ion source voltage 1	20 kV
Ion source voltage 2	19.01 kV
Lens voltage	5 kV
Linear detector voltage	1.44 kV
Reflector voltage 1	0 kV
Reflector voltage 2	0 kV
Reflector detector voltage	1.569 kV

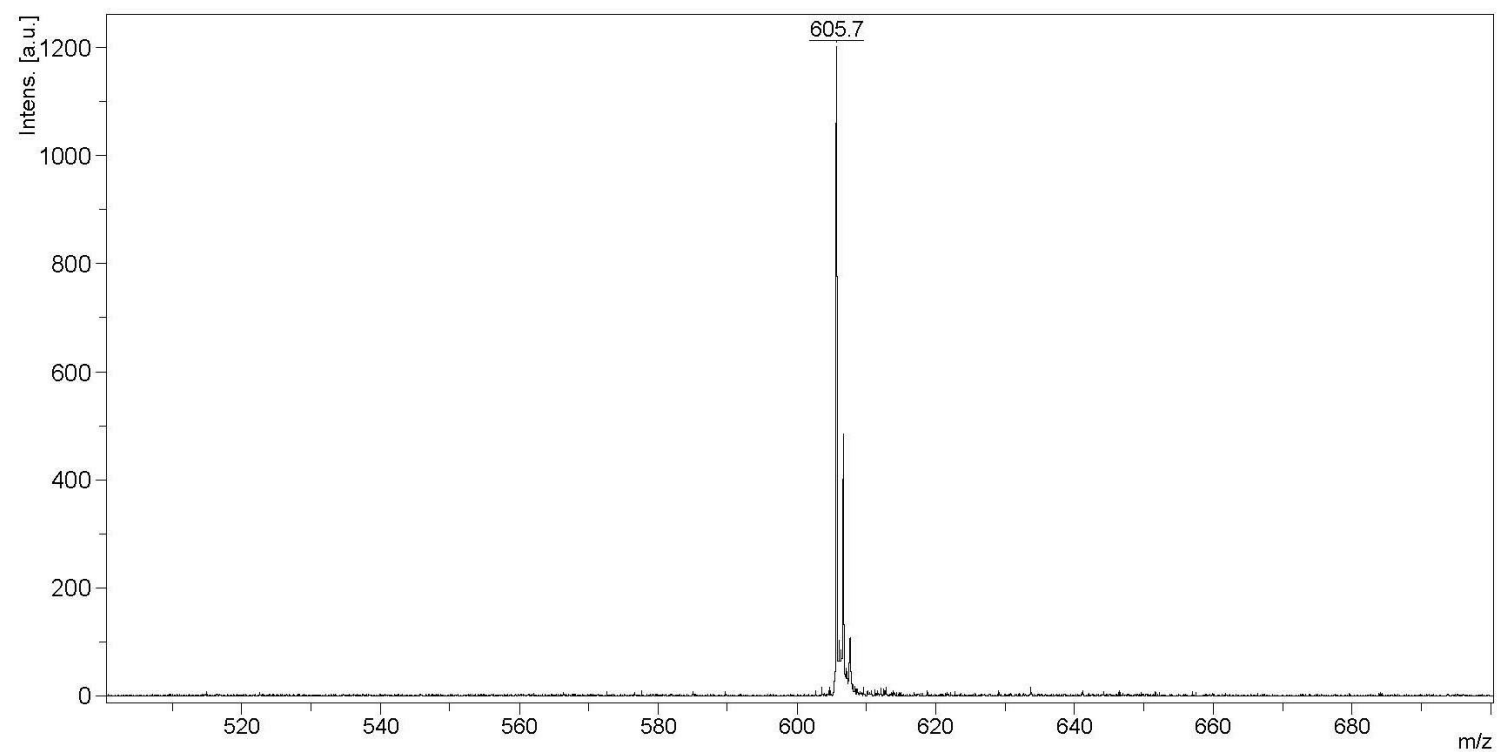
Laser

Ion Source Type	MALDI
Laser Type	Nd:YAG
Wavelength	355 nm
Number of shots	50
Laser repetition rate	100 Hz

Target

Target Plate	MTP AnchorChip
Position	K20

Figure S98. MALDI spectrum of compound **3a**

**Instrument**

Instrument type	ultraflexTOF/TOF
Name of computer	MALDI
flexControl version	flexControl 3.0.173.0
flexAnalysis version	3.0.96.0

Spectrometer

Ion Polarity	POS
PIE delay	50 ns
Ion source voltage 1	20 kV
Ion source voltage 2	19.01 kV
Lens voltage	5 kV
Linear detector voltage	1.44 kV
Reflector voltage 1	0 kV
Reflector voltage 2	0 kV
Reflector detector voltage	0 kV

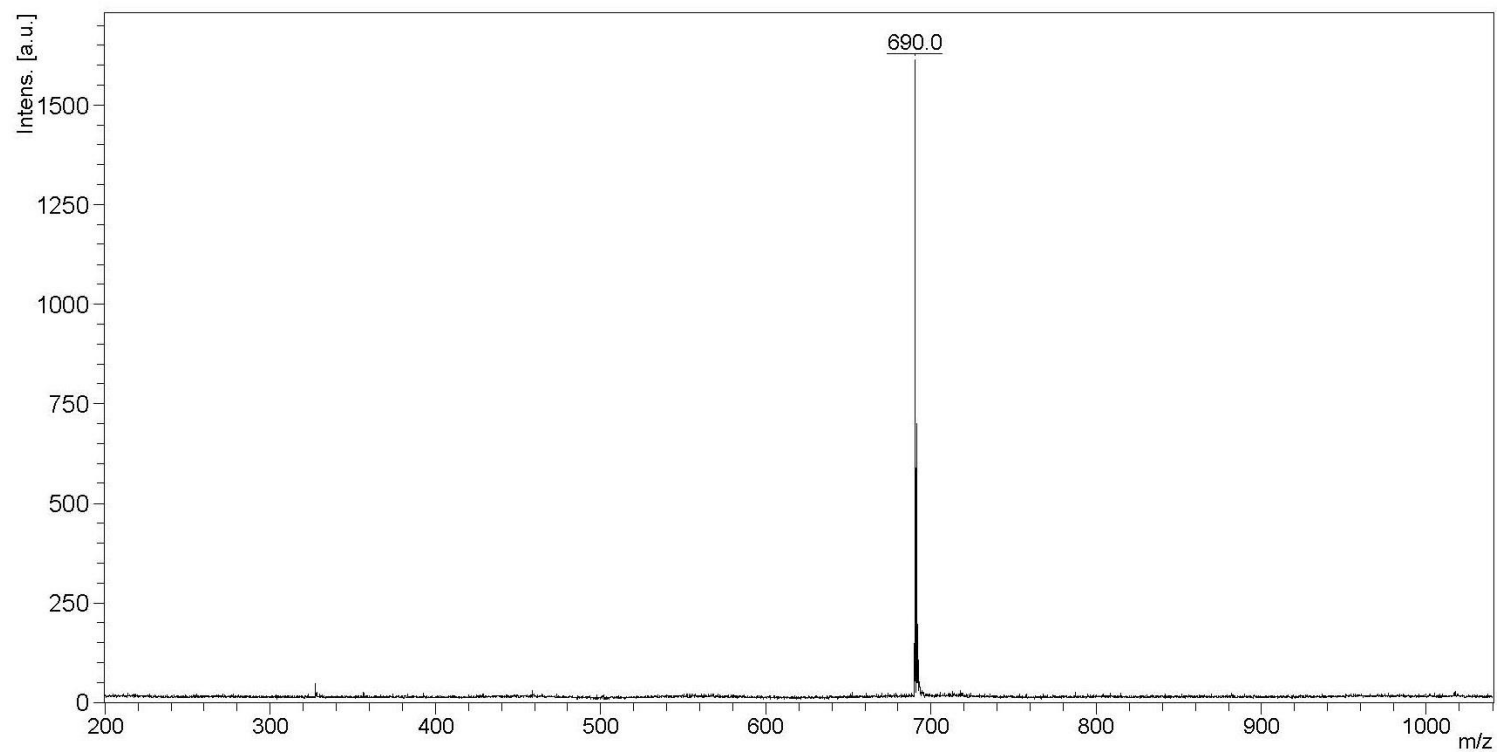
Laser

Ion Source Type	MALDI
Laser Type	Nd:YAG
Wavelength	355 nm
Number of shots	150
Laser repetition rate	100 Hz

Target

Target Plate	MTP AnchorChip
Position	J1

Figure S99. MALDI spectrum of compound **3b**



Instrument

Instrument type	ultraflexTOF/TOF
Name of computer	MALDI
flexControl version	flexControl 3.0.173.0
flexAnalysis version	3.0.96.0

Spectrometer

Ion Polarity	POS
PIE delay	30 ns
Ion source voltage 1	20 kV
Ion source voltage 2	19.01 kV
Lens voltage	5 kV
Linear detector voltage	1.44 kV
Reflector voltage 1	0 kV
Reflector voltage 2	0 kV
Reflector detector voltage	1.569 kV

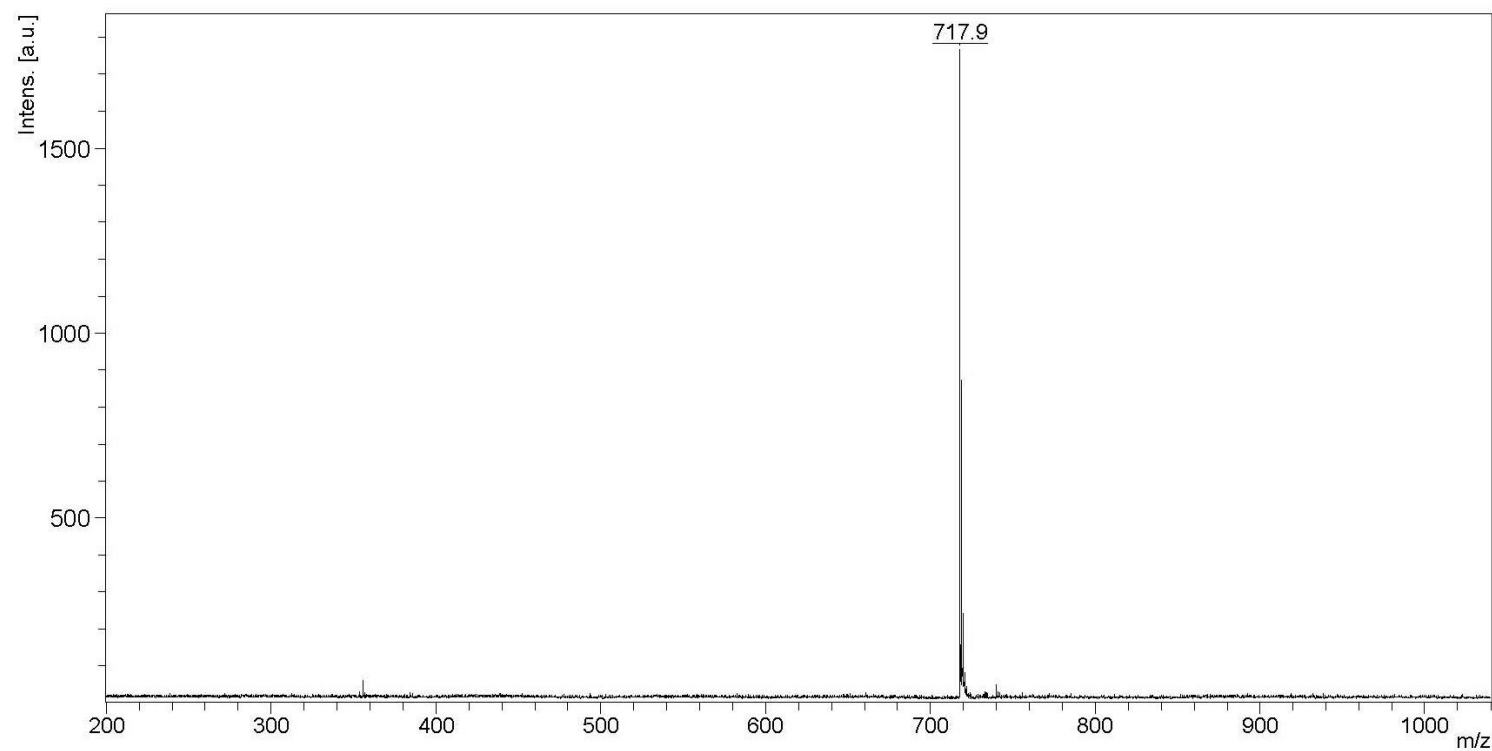
Laser

Ion Source Type	MALDI
Laser Type	Nd:YAG
Wavelength	355 nm
Number of shots	50
Laser repetition rate	100 Hz

Target

Target Plate	MTP AnchorChip
Position	N19

Figure S100. MALDI spectrum of compound **3c**



Instrument

Instrument type	ultraflexTOF/TOF
Name of computer	MALDI
flexControl version	flexControl 3.0.173.0
flexAnalysis version	3.0.96.0

Spectrometer

Ion Polarity	POS
PIE delay	30 ns
Ion source voltage 1	20 kV
Ion source voltage 2	19.01 kV
Lens voltage	5 kV
Linear detector voltage	1.44 kV
Reflector voltage 1	0 kV
Reflector voltage 2	0 kV
Reflector detector voltage	1.569 kV

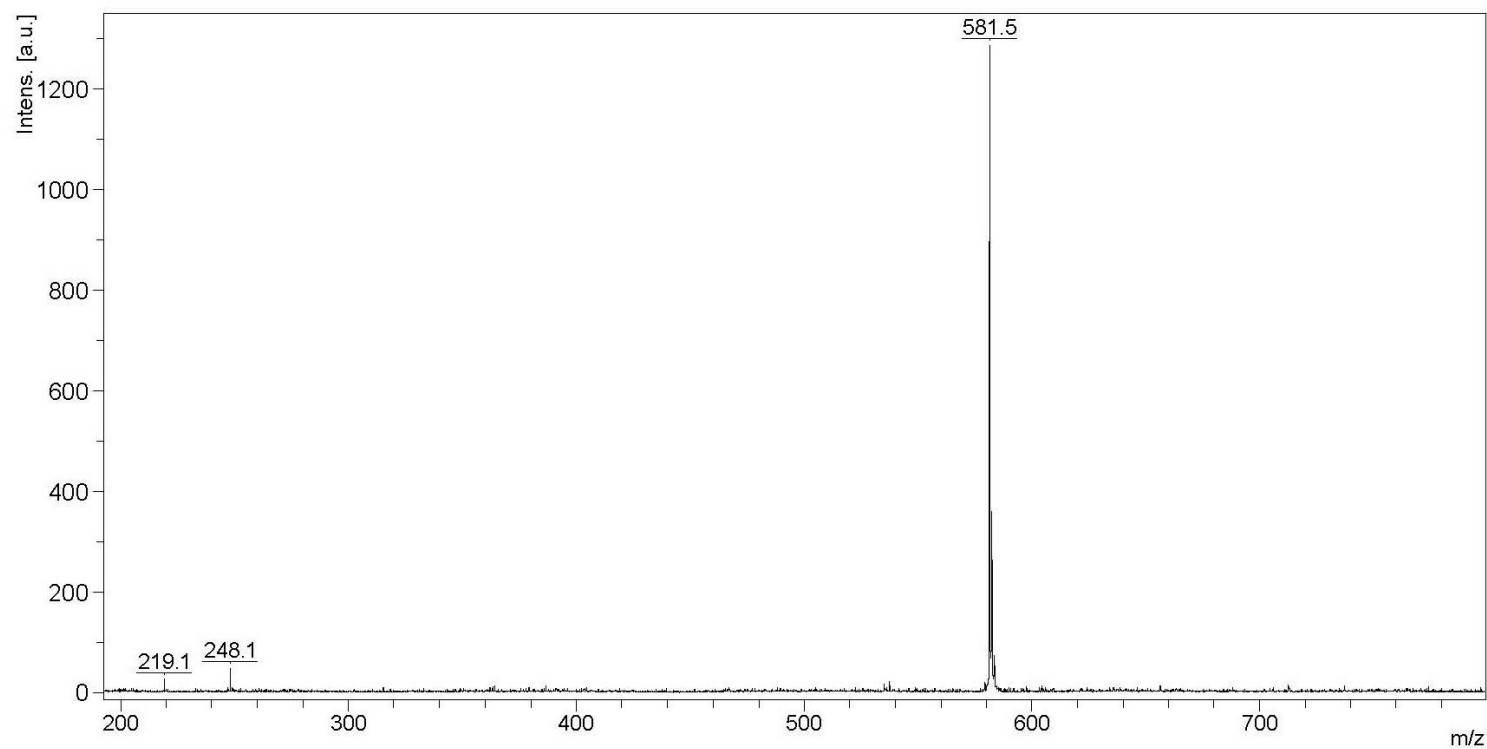
Laser

Ion Source Type	MALDI
Laser Type	Nd:YAG
Wavelength	355 nm
Number of shots	50
Laser repetition rate	100 Hz

Target

Target Plate	MTP AnchorChip
Position	N20

Figure S101. MALDI spectrum of compound **3d**



Instrument

Instrument type	ultraflexTOF/TOF
Name of computer	MALDI
flexControl version	flexControl 3.0.173.0
flexAnalysis version	3.0.96.0

Spectrometer

Ion Polarity	POS
PIE delay	30 ns
Ion source voltage 1	20 kV
Ion source voltage 2	19.01 kV
Lens voltage	5 kV
Linear detector voltage	1.44 kV
Reflector voltage 1	0 kV
Reflector voltage 2	0 kV
Reflector detector voltage	1.569 kV

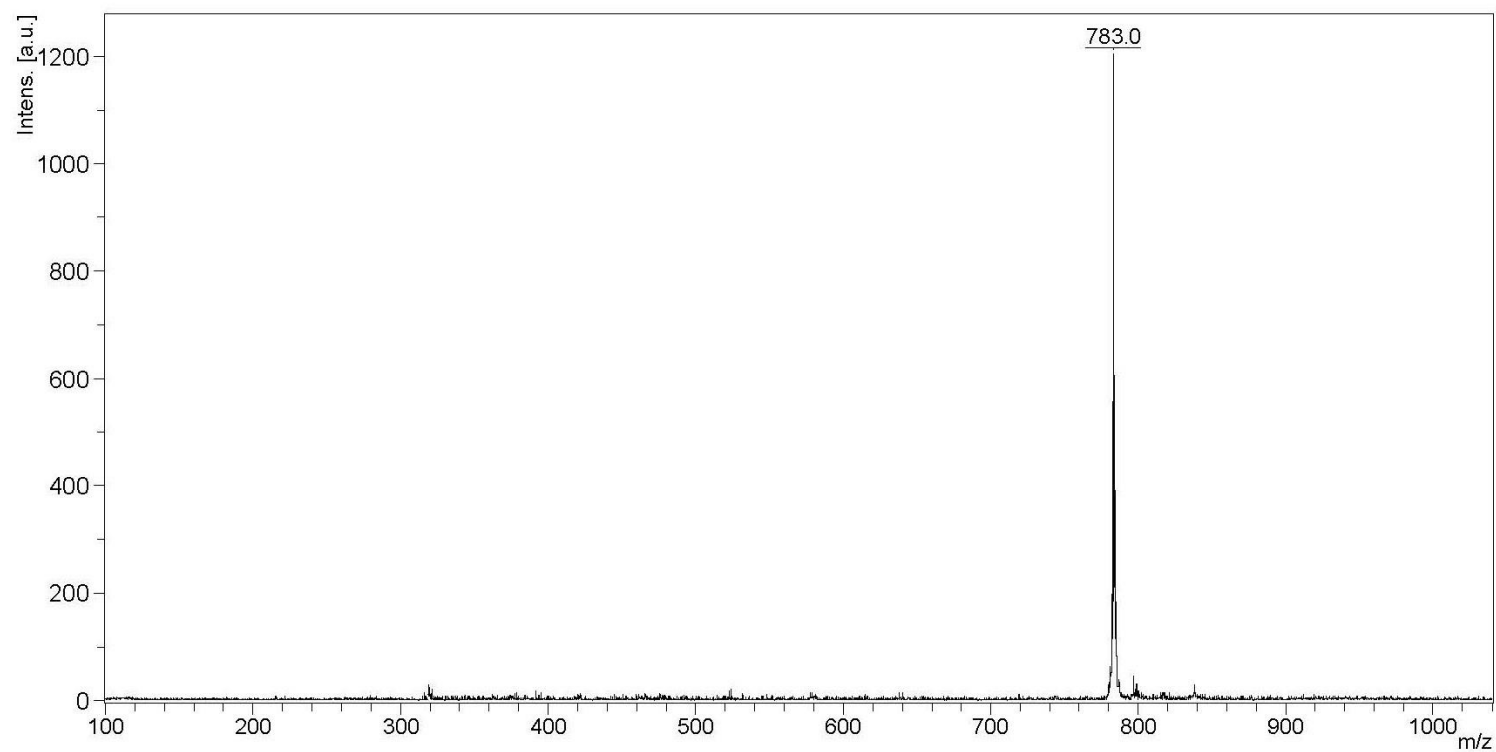
Laser

Ion Source Type	MALDI
Laser Type	Nd:YAG
Wavelength	355 nm
Number of shots	50
Laser repetition rate	100 Hz

Target

Target Plate	MTP AnchorChip
Position	K24

Figure S102. MALDI spectrum of compound **3e**



Instrument

Instrument type	ultraflexTOF/TOF
Name of computer	MALDI
flexControl version	flexControl 3.0.173.0
flexAnalysis version	3.0.96.0

Spectrometer

Ion Polarity	POS
PIE delay	30 ns
Ion source voltage 1	20 kV
Ion source voltage 2	19.01 kV
Lens voltage	5 kV
Linear detector voltage	1.44 kV
Reflector voltage 1	0 kV
Reflector voltage 2	0 kV
Reflector detector voltage	0 kV

Laser

Ion Source Type	MALDI
Laser Type	Nd:YAG
Wavelength	355 nm
Number of shots	50
Laser repetition rate	66.667 Hz

Target

Target Plate	MTP AnchorChip
Position	G5

Figure S103. MALDI spectrum of compound **3f**

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	100 m/z	Scan End	2000 m/z
Capillary Exit	140.0 V	n/a	n/a	Trap Drive	58.1
Accumulation Time	831 μ s	Averages	5 Spectra	n/a	n/a

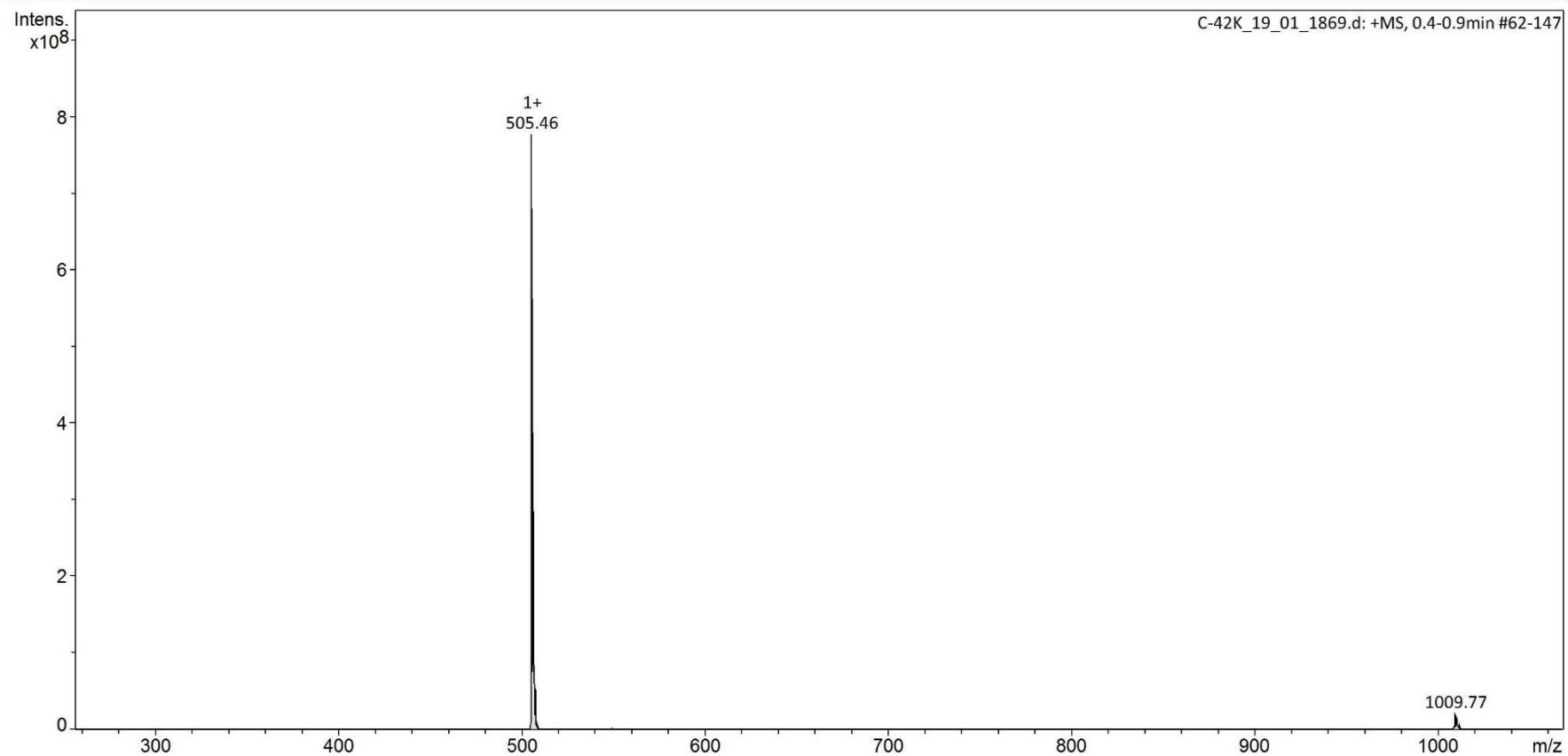
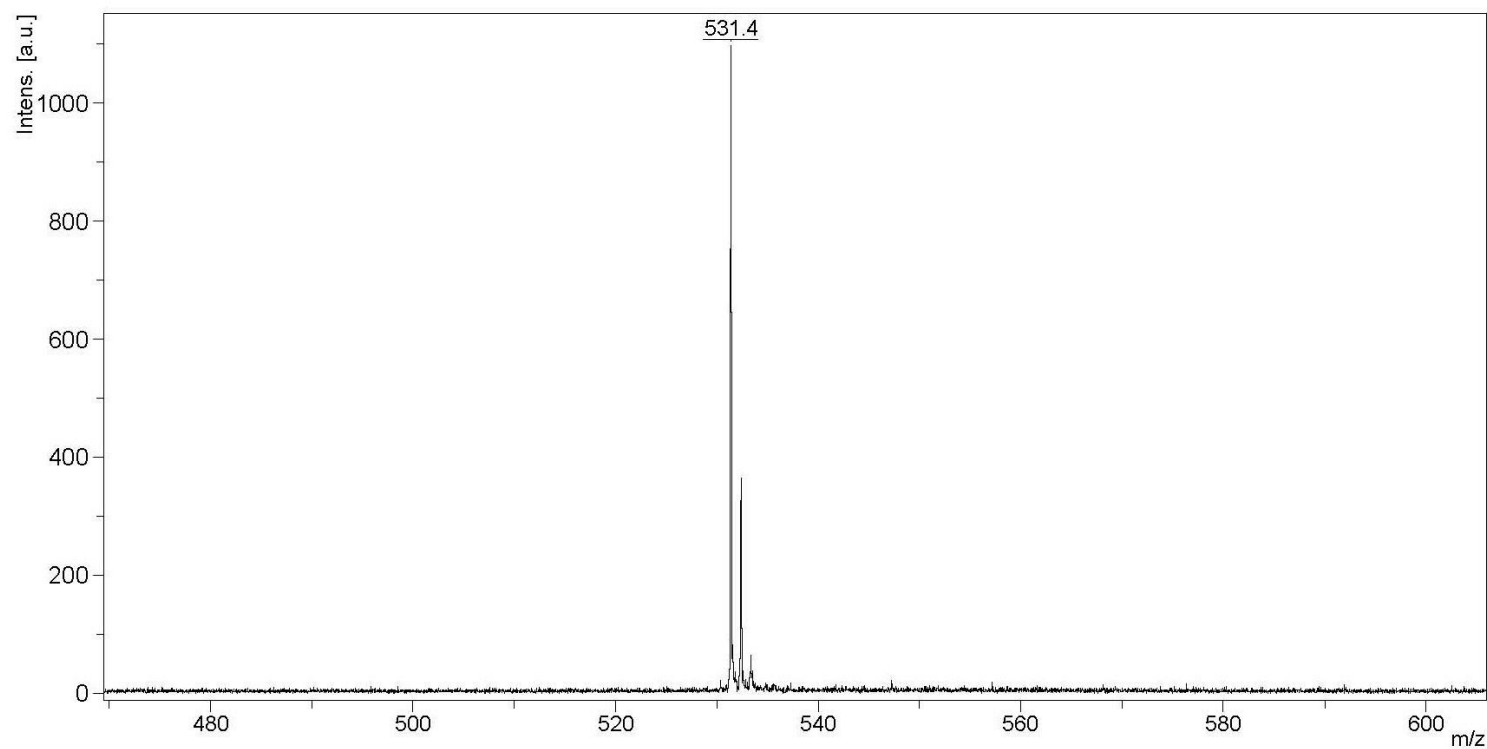


Figure S104. ESI spectrum of compound **3g**



Instrument

Instrument type	ultraflexTOF/TOF
Name of computer	MALDI
flexControl version	flexControl 3.0.173.0
flexAnalysis version	3.0.96.0

Spectrometer

Ion Polarity	POS
PIE delay	30 ns
Ion source voltage 1	20 kV
Ion source voltage 2	19.01 kV
Lens voltage	5 kV
Linear detector voltage	1.44 kV
Reflector voltage 1	0 kV
Reflector voltage 2	0 kV
Reflector detector voltage	1.569 kV

Laser

Ion Source Type	MALDI
Laser Type	Nd:YAG
Wavelength	355 nm
Number of shots	150
Laser repetition rate	100 Hz

Target

Target Plate	MTP AnchorChip
Position	K23

Figure S105. MALDI spectrum of compound **3h**

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	100 m/z	Scan End	2000 m/z
Capillary Exit	140.0 V	n/a	n/a	Trap Drive	58.1
Accumulation Time	1300 μ s	Averages	5 Spectra	n/a	n/a

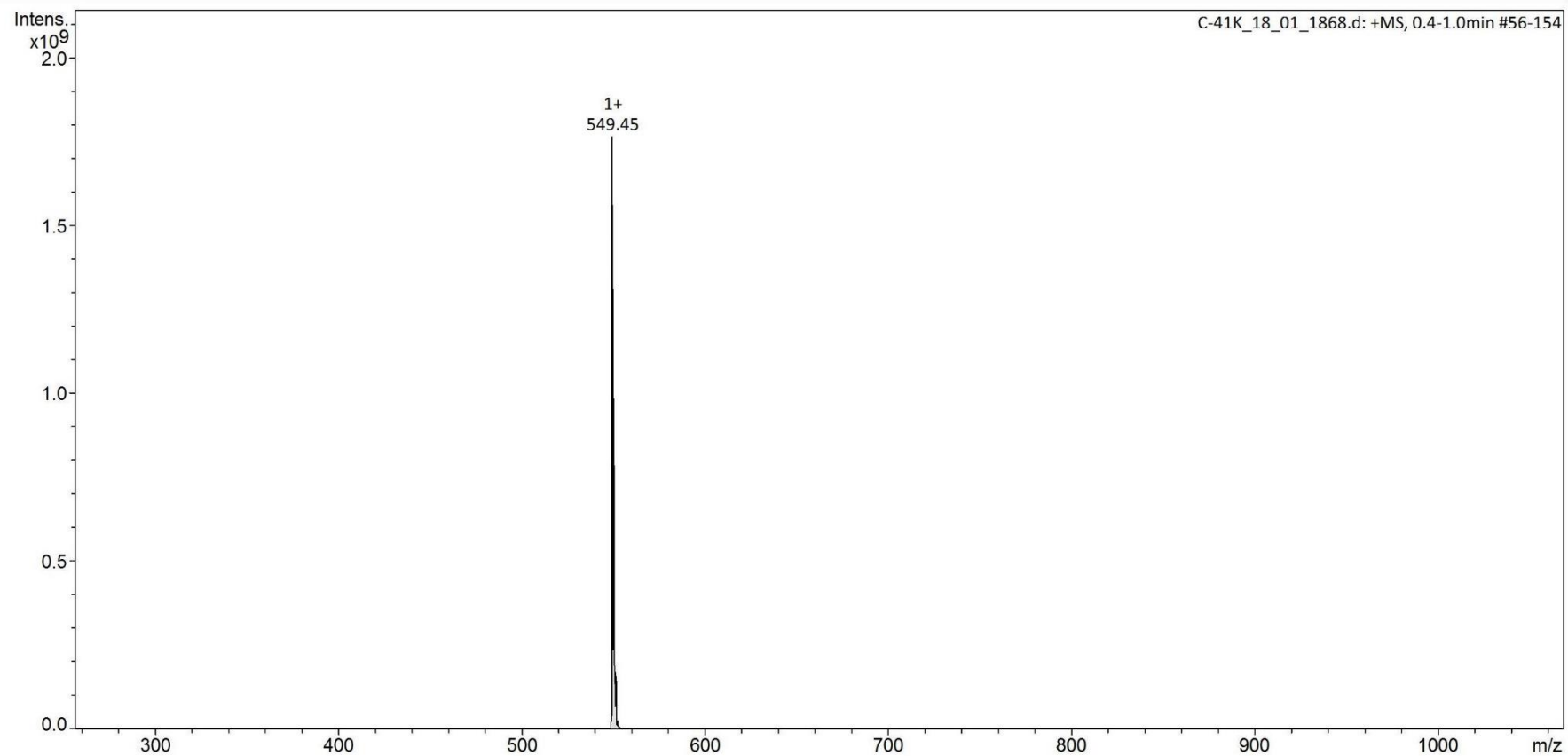


Figure S106. ESI spectrum of compound **3i**

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	200 m/z	Scan End	2800 m/z
Capillary Exit	140.0 V	n/a	n/a	Trap Drive	73.1
Accumulation Time	268 μ s	Averages	5 Spectra	n/a	n/a

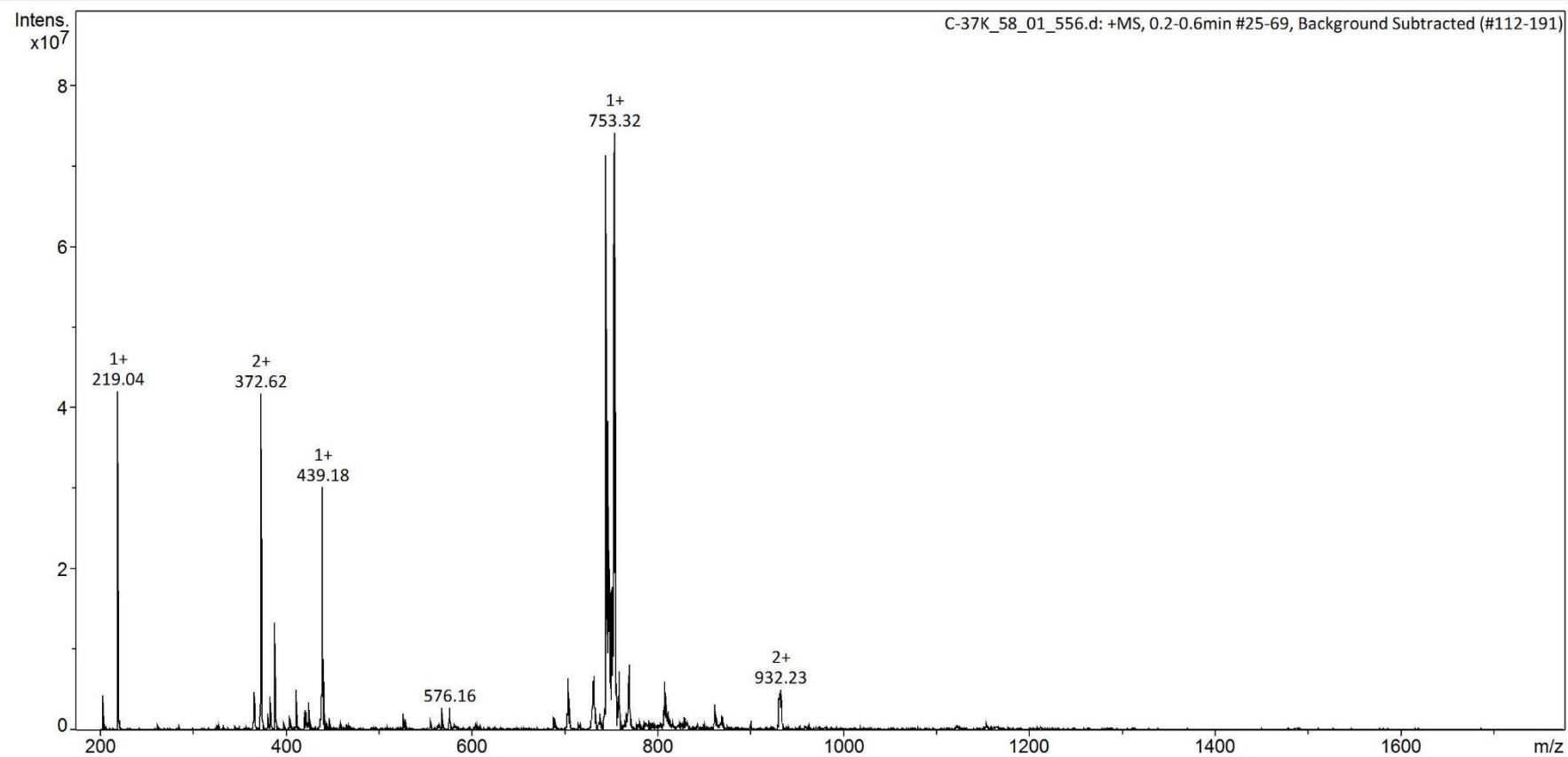
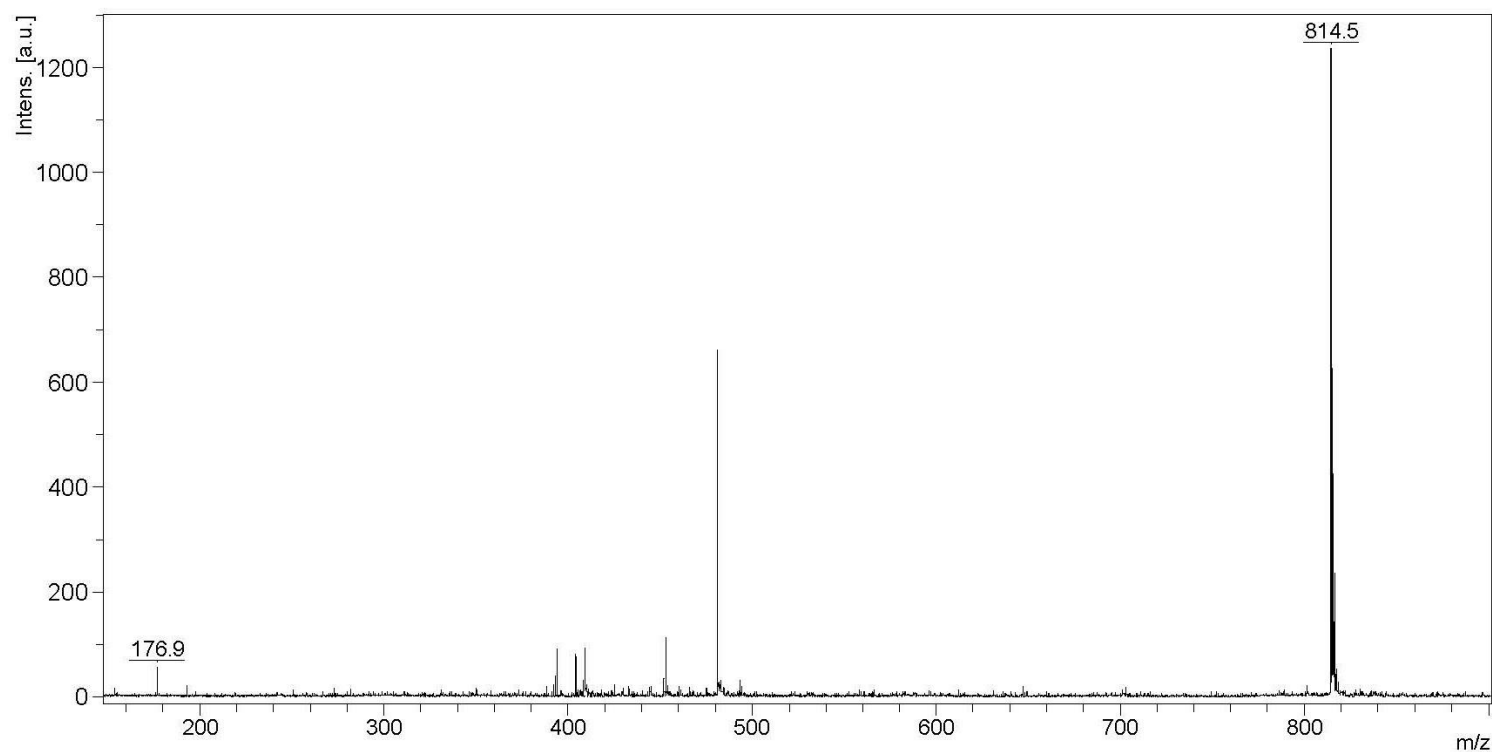


Figure S107. ESI spectrum of compound **3j**



Instrument

Instrument type: ultraflexTOF/TOF
 Name of computer: MALDI
 flexControl version: flexControl 3.0.173.0
 flexAnalysis version: 3.0.96.0

Spectrometer

Ion Polarity: POS
 PIE delay: 30 ns
 Ion source voltage 1: 20 kV
 Ion source voltage 2: 19.01 kV
 Lens voltage: 5 kV
 Linear detector voltage: 1.44 kV
 Reflector voltage 1: 0 kV
 Reflector voltage 2: 0 kV
 Reflector detector voltage: 1.569 kV

Laser

Ion Source Type: MALDI
 Laser Type: Nd:YAG
 Wavelength: 355 nm
 Number of shots: 50
 Laser repetition rate: 100 Hz

Target

Target Plate: MTP AnchorChip
 Position: K21

Figure S108. MALDI spectrum of compound **3k**

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	70 m/z	Scan End	2700 m/z
Capillary Exit	140.0 V	n/a	n/a	Trap Drive	73.1
Accumulation Time	556 μ s	Averages	5 Spectra	Auto MS/MS	off

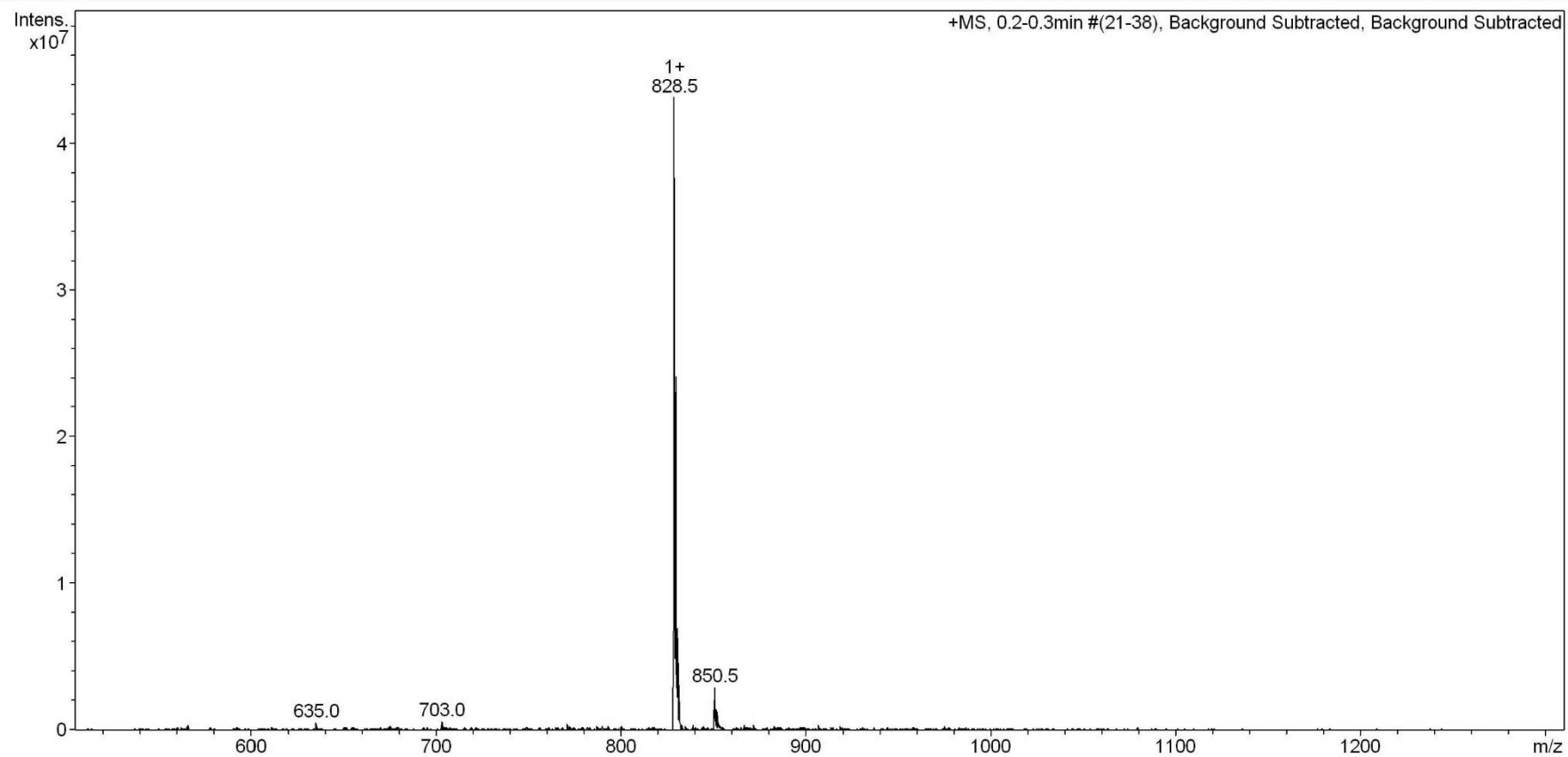


Figure S109. ESI spectrum of compound **3I**

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	70 m/z	Scan End	2700 m/z
Capillary Exit	140.0 V	n/a	n/a	Trap Drive	73.1
Accumulation Time	543 μ s	Averages	5 Spectra	Auto MS/MS	off

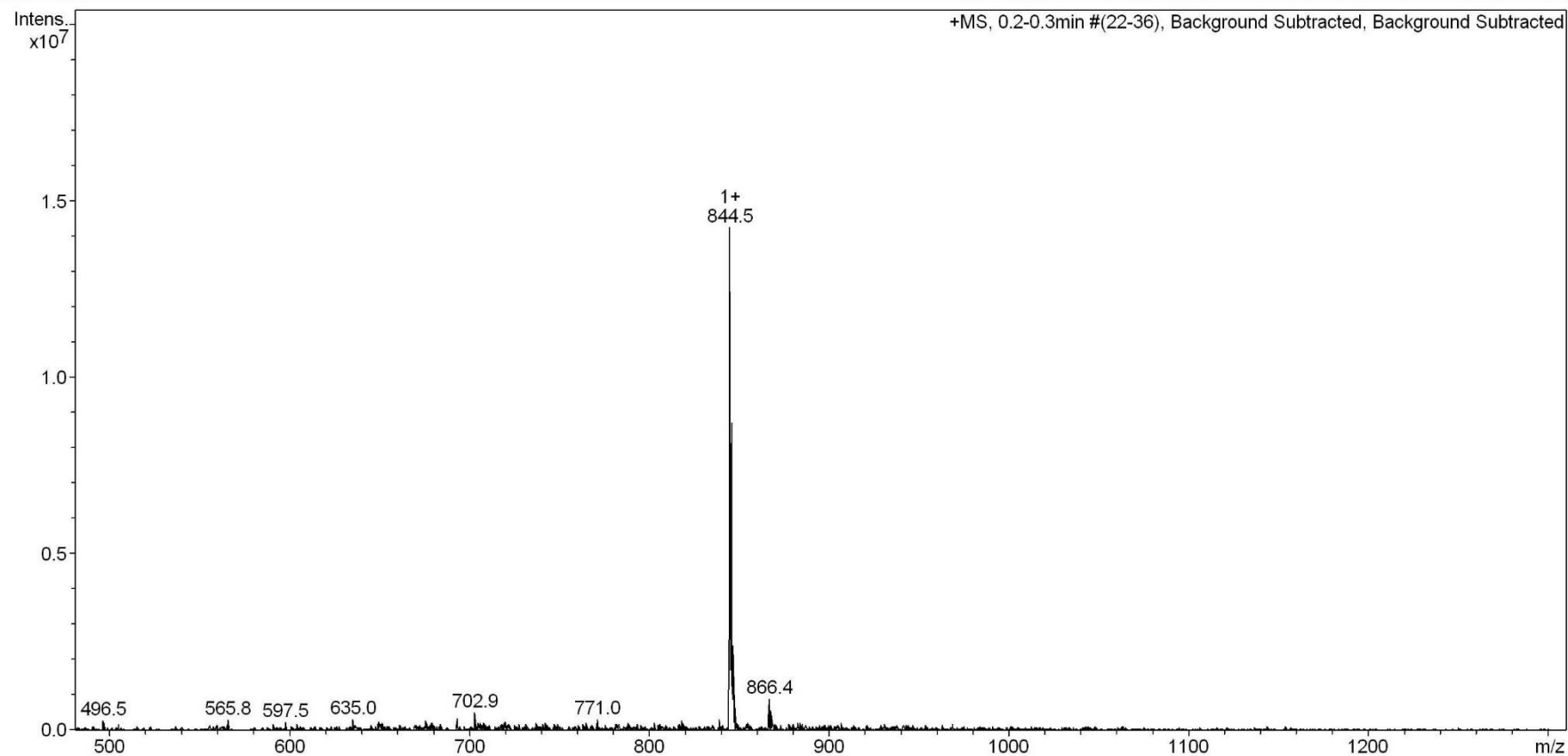
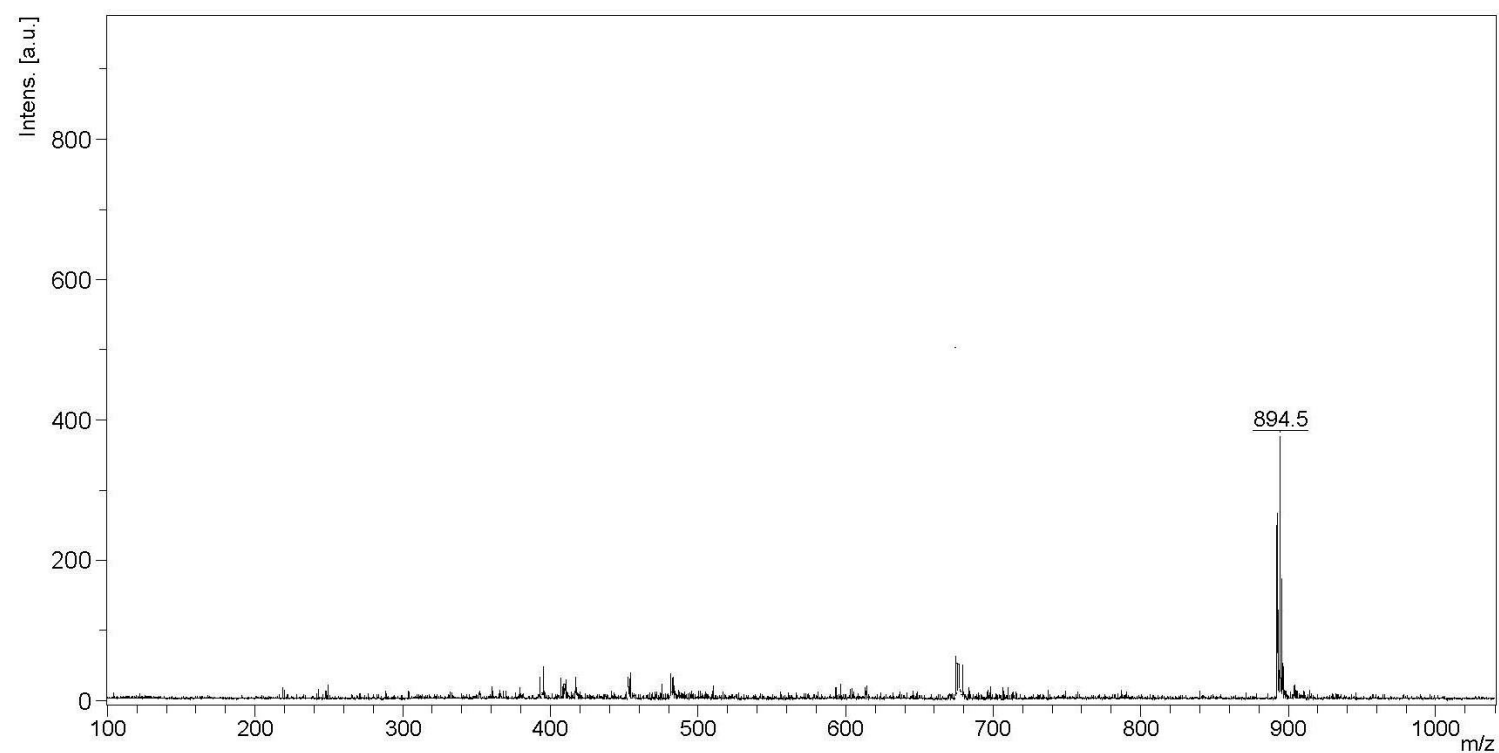


Figure S110. ESI spectrum of compound **3m**

**Instrument**

Instrument type	ultraflexTOF/TOF
Name of computer	MALDI
flexControl version	flexControl 3.0.173.0
flexAnalysis version	3.0.96.0

Spectrometer

Ion Polarity	POS
PIE delay	30 ns
Ion source voltage 1	20 kV
Ion source voltage 2	19.01 kV
Lens voltage	5 kV
Linear detector voltage	1.44 kV
Reflector voltage 1	0 kV
Reflector voltage 2	0 kV
Reflector detector voltage	1.569 kV

Laser

Ion Source Type	MALDI
Laser Type	Nd:YAG
Wavelength	355 nm
Number of shots	100
Laser repetition rate	100 Hz

Target

Target Plate	MTP AnchorChip
Position	J18

Figure S111. MALDI spectrum of compound **3n**