Chemistry and Folding of Photomodulable Peptides - Stilbene and Thioaurone-type Candidates for Conformational Switches

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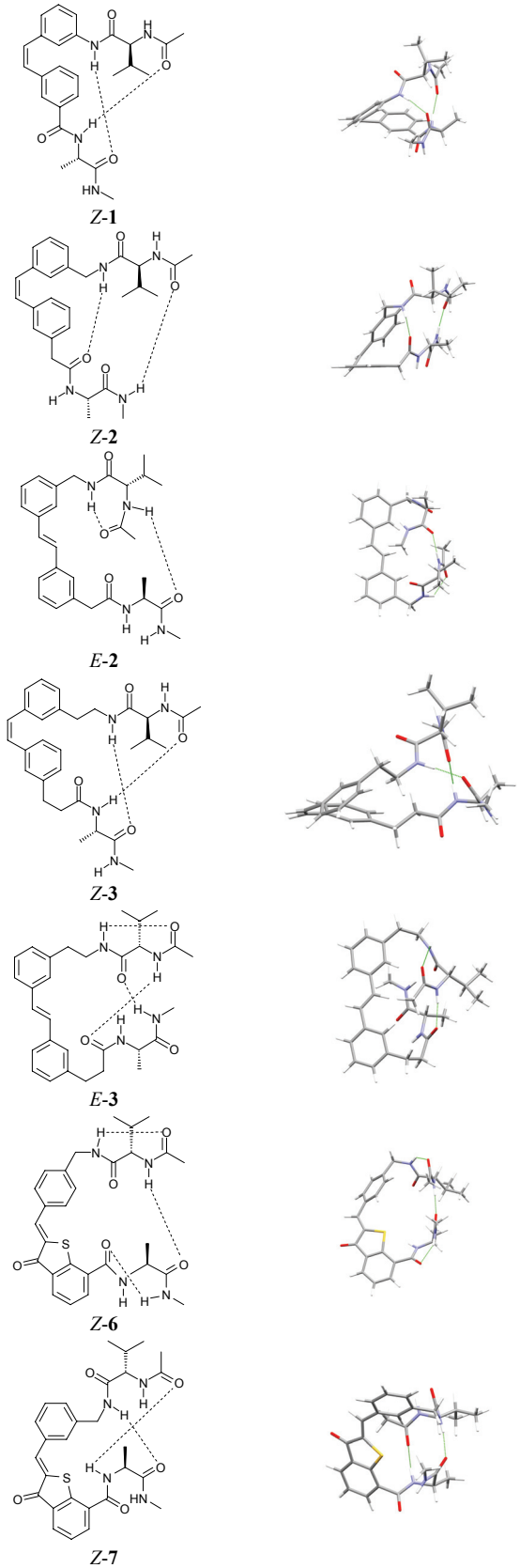
Table S1 Amide proton temperature coefficients (ppb/K) in DMSO-d_6, CH_3OH:CD_3OD (1:1), H_2O:D_2O (1:1), and $CDCl_3$ solution.

Residue	**DMSO**	**MeOH**	**DMSO**	**MeOH**
	trans-1		**cis-1**	
$NH^{Ph/Gly}$	5.2	6.3	5.1	6.8
NH^{CH3}	4.4	6.6	4.2	6.9
NH^{Ala}	4.9	6.9	5.7	9.0
NH^{Val}	5.7	7.1	5.9	7.4
	trans-2		**cis-2**	
$NH^{Ph/CH2}$	5.2	7.1	6.5	7.4
NH^{CH3}	5.1	7.5	7.1	7.8
NH^{Ala}	6.0	9.1	8.6	9.9
NH^{Val}	5.4	7.7	7.2	9.4
	trans-3		**cis-3**	
$NH^{Ph/CH2}$	5.5	7.5	5.7	8.2
NH^{CH3}	5.6	7.5	5.3	7.6
NH^{Ala}	5.7	7.2	5.6	8.7
NH^{Val}	5.3	7.8	5.8	8.3
	Z-4, DMSO		**E-4**, **DMSO**	
NH^{Ala}	4.7		4.7	
NH^{thio}	5.2		5.1	
NH^{Val}	5.5		7.3	
	Z-5, DMSO		**E-5**, **DMSO**	
NH^{Ala}	4.7		4.7	
NH^{thio}	5.2		5.3	
NH^{Val}	5.4		5.1	
	Z-6, DMSO		**E-6**, **DMSO**	
NH^{Ala}	5.1		5.1	
NH^{thio}	5.2		5.8	
NH^{Val}	5.5		5.6	
NH^{Cap}	4.4		4.5	
	Z-7, DMSO		**E-7**, **DMSO**	
NH^{Ala}	5.1		4.9	
NH^{thio}	5.2		5.5	
NH^{Val}	5.5		5.0	
NH^{Cap}	4.5		4.5	
	DMSO	**MeOH**	**H_2O**	**$CDCl_3$**
	8			
NH^{Gly}	4.2	6.5	5.5	5.7
NH^{CH3}	3.8	3.6	5.5	7.3
NH^{Ala}	3.2	3.4	5.1	7.2
NH^{Val}	5.0	6.1	2.0	6.8
	10			
NH^{Ph-CH2}	5.6	Many confor-mations		
NH^{CH3}	4.8			
NH^{Ala}	6.8			
NH^{Val}	6.0			



Z-**1**

Z-**2**

E-**2**

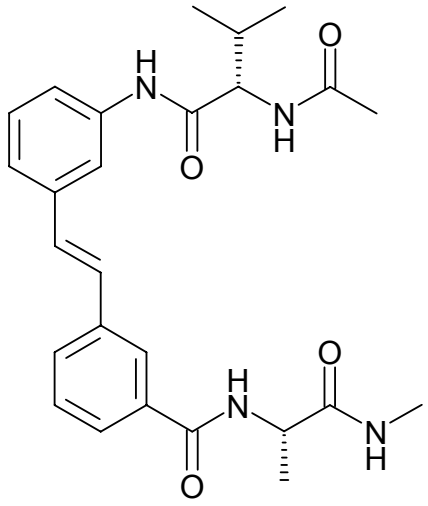
Z-**3**

E-**3**

Z-**6**

Z-**7**

Scheme S1. Hydrogen bonds (dashed lines in structure formulae, green dashed lines in modelled figures) in selected low energy conformers of the photoswitchable petidomimetics. Structure formulae are drawn to show the hydrogen bonds, not the spatial arrangement. For clarity, only a single low-energy conformer is shown.



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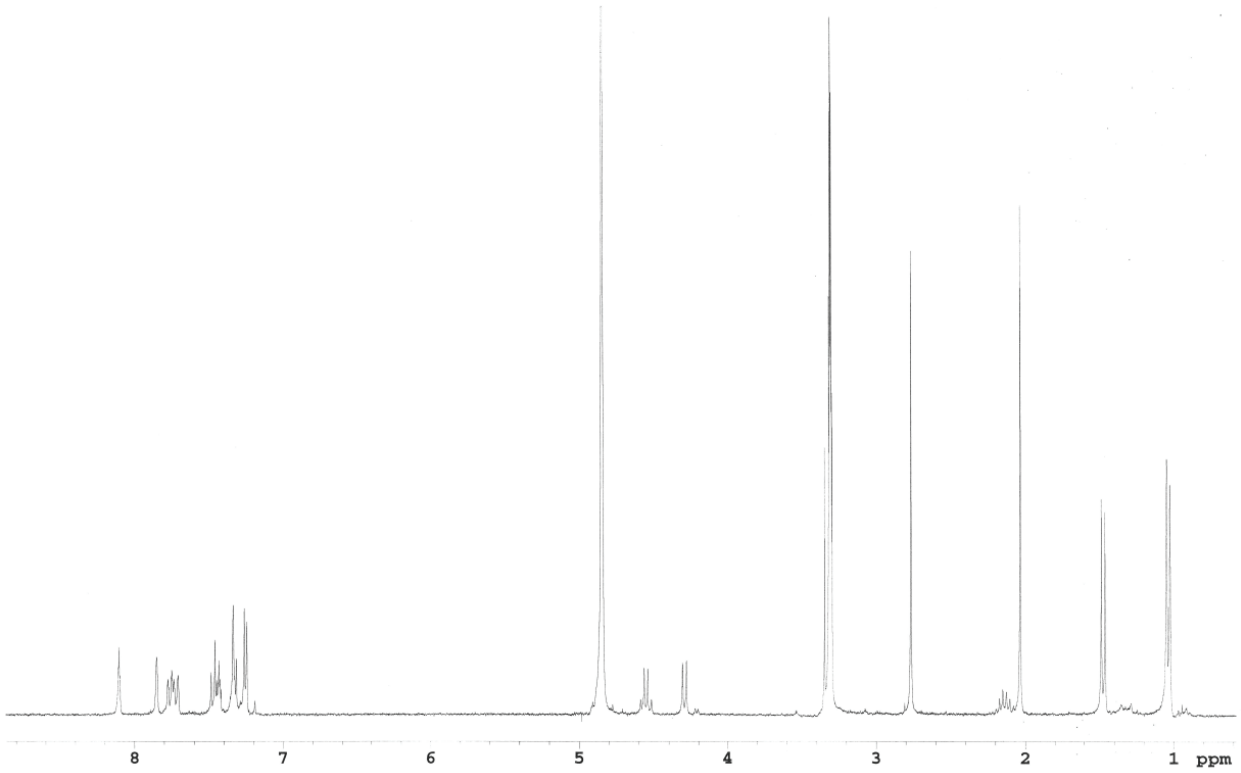

Figure S 1: ^{1}H NMR spectrum of compound **E-1** (300.0 MHz, CD_3OD/CH_3OH (1:1) solution, 25°C).

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Figure S 2: ^{1}H NMR spectrum of compound **E-2** (499.9 MHz, CD_3OD/CH_3OH (1:1) solution, solvent suppression used, 25°C).

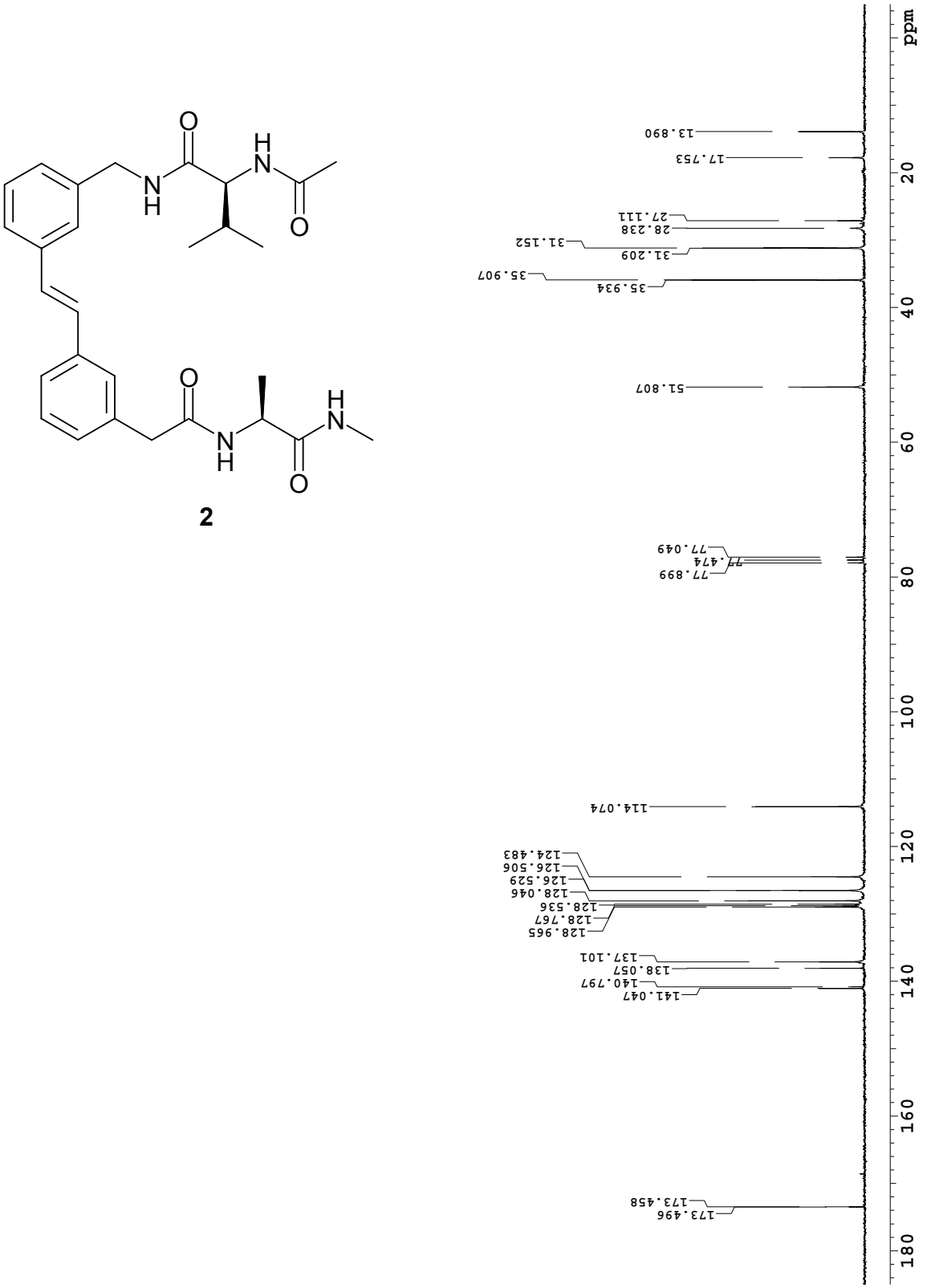

Figure S 3: ^{13}C NMR spectrum of compound **E-2** (75 MHz, CD_3OD/CH_3OH (1:1) solution, 25°C).

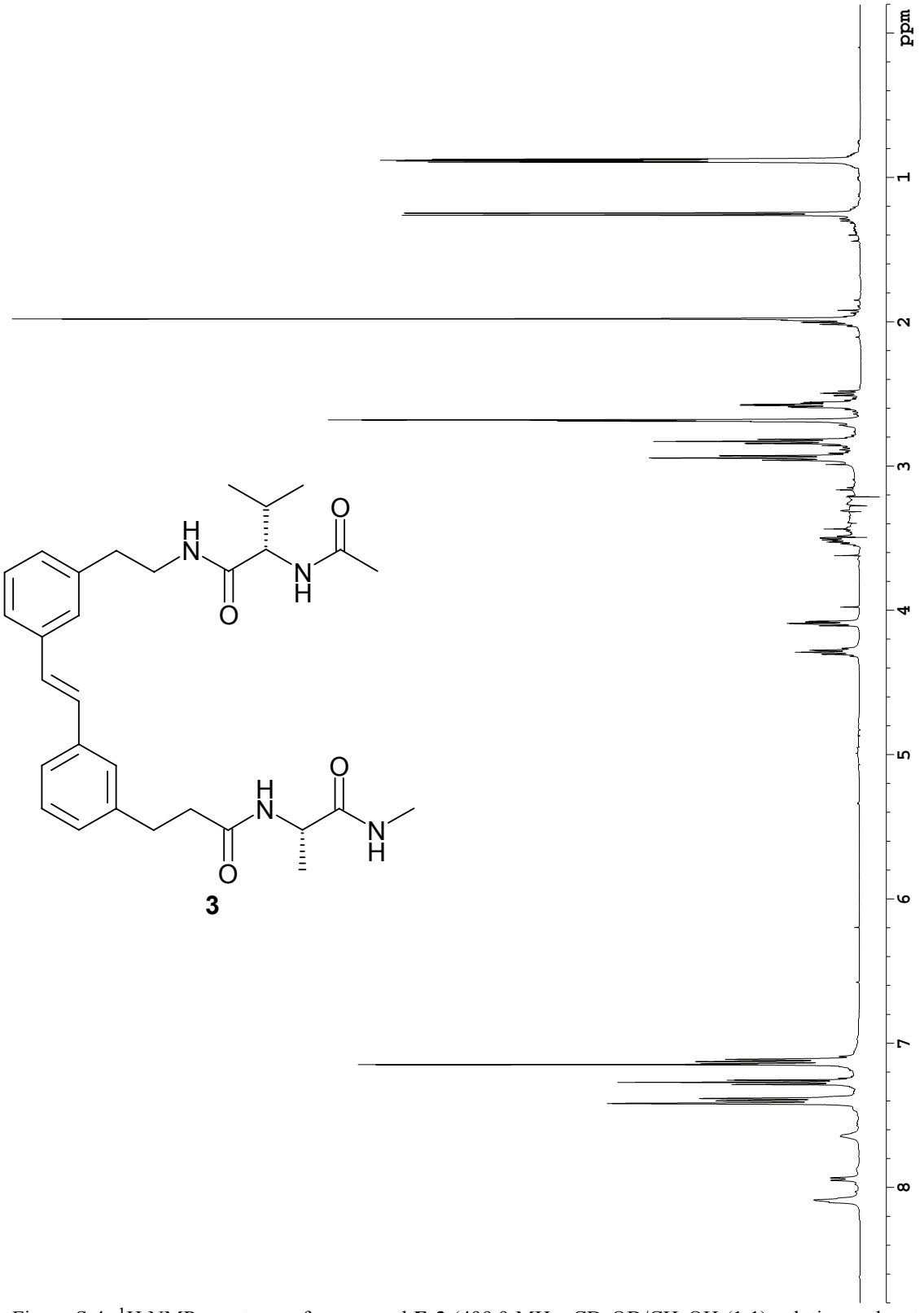

Figure S 4: ^{1}H NMR spectrum of compound **E-3** (499.9 MHz, CD_3OD/CH_3OH (1:1) solution, solvent suppression used, 25°C).

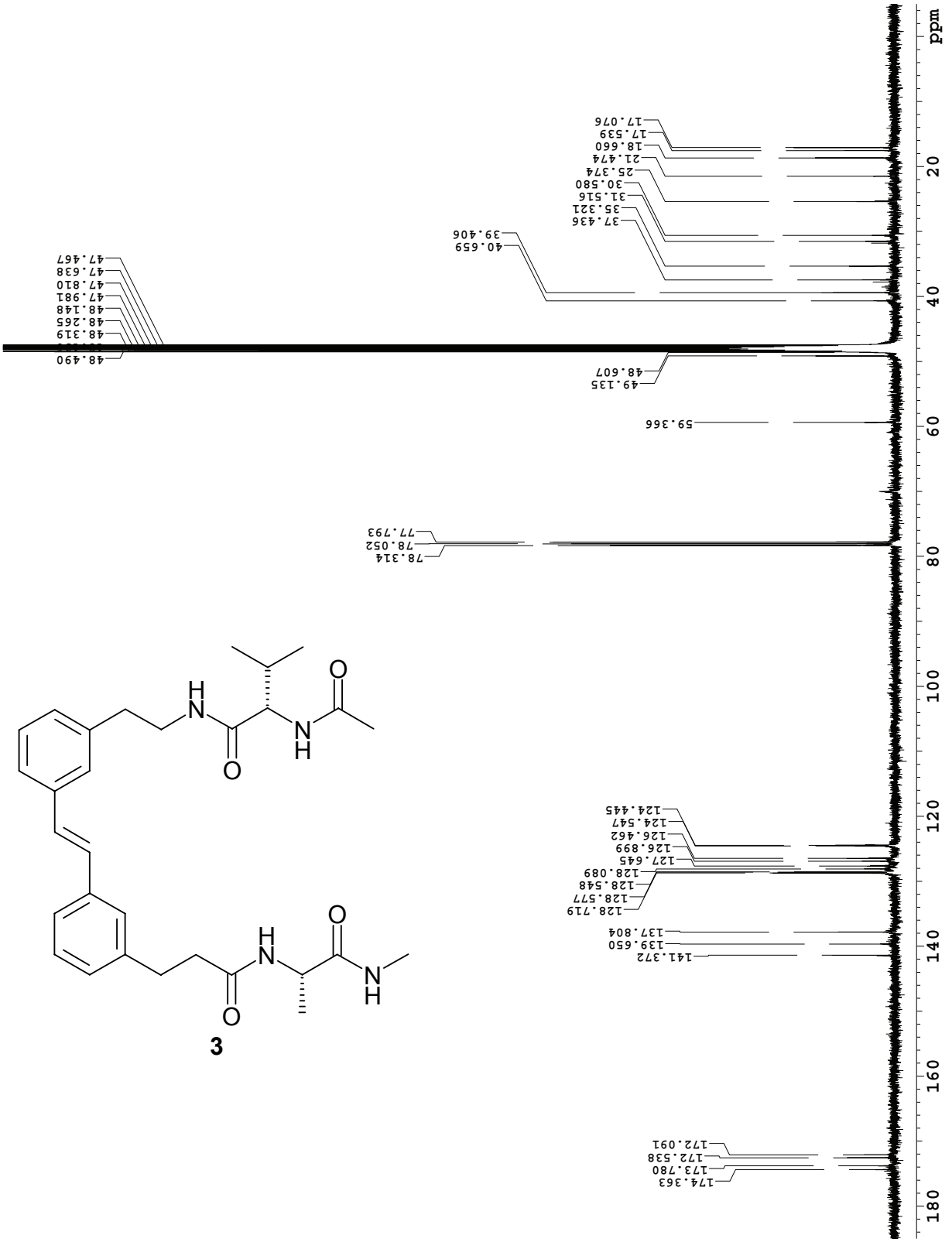

Figure S 5: ^{13}C NMR spectrum of compound **E-3** (75 MHz, CD_3OD/CH_3OH (1:1) solution, 25°C).

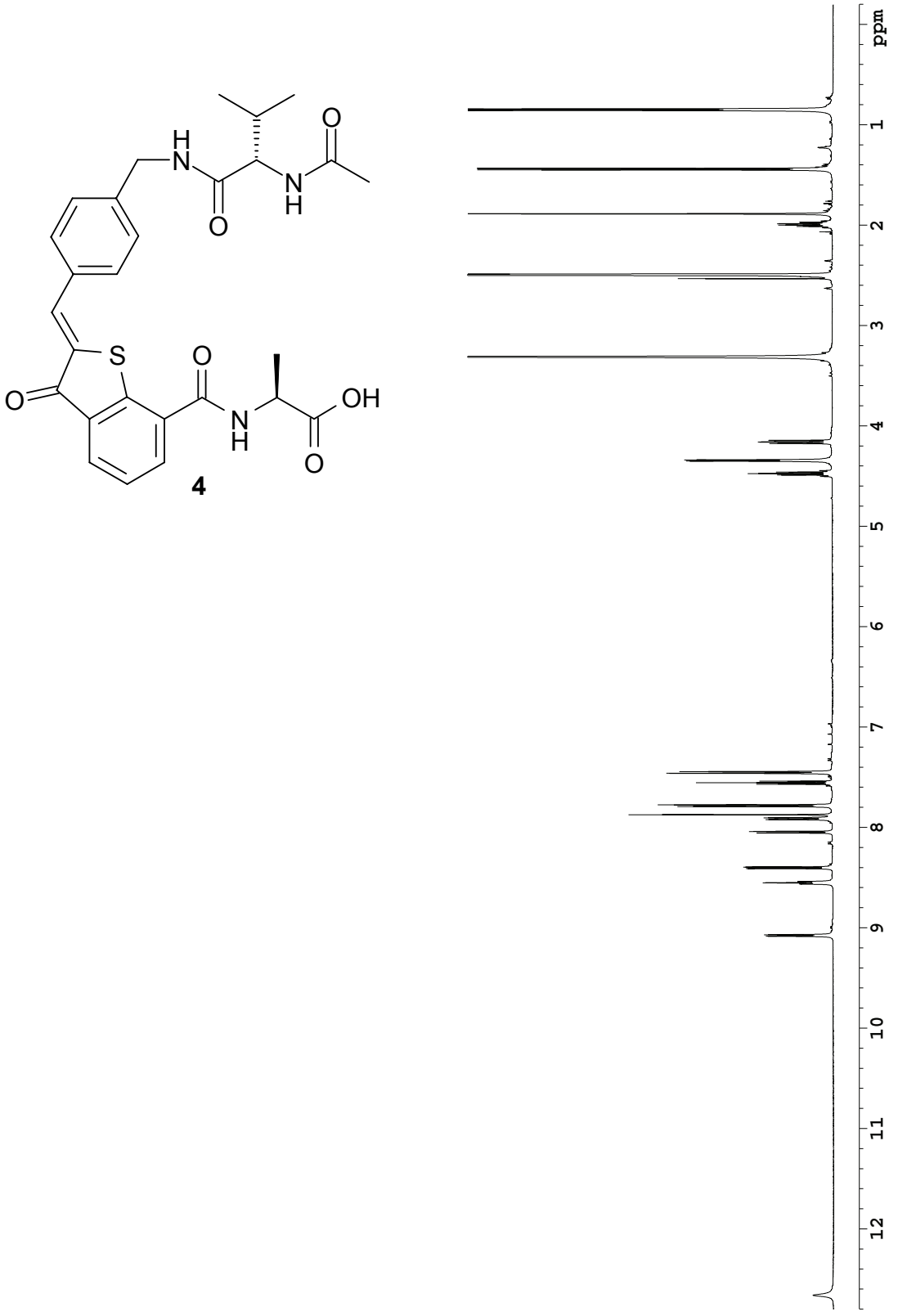

Figure S 6: ^{1}H NMR spectrum of compound **Z-4** (499.9 MHz, DMSO-d_6 solution, 25°C).

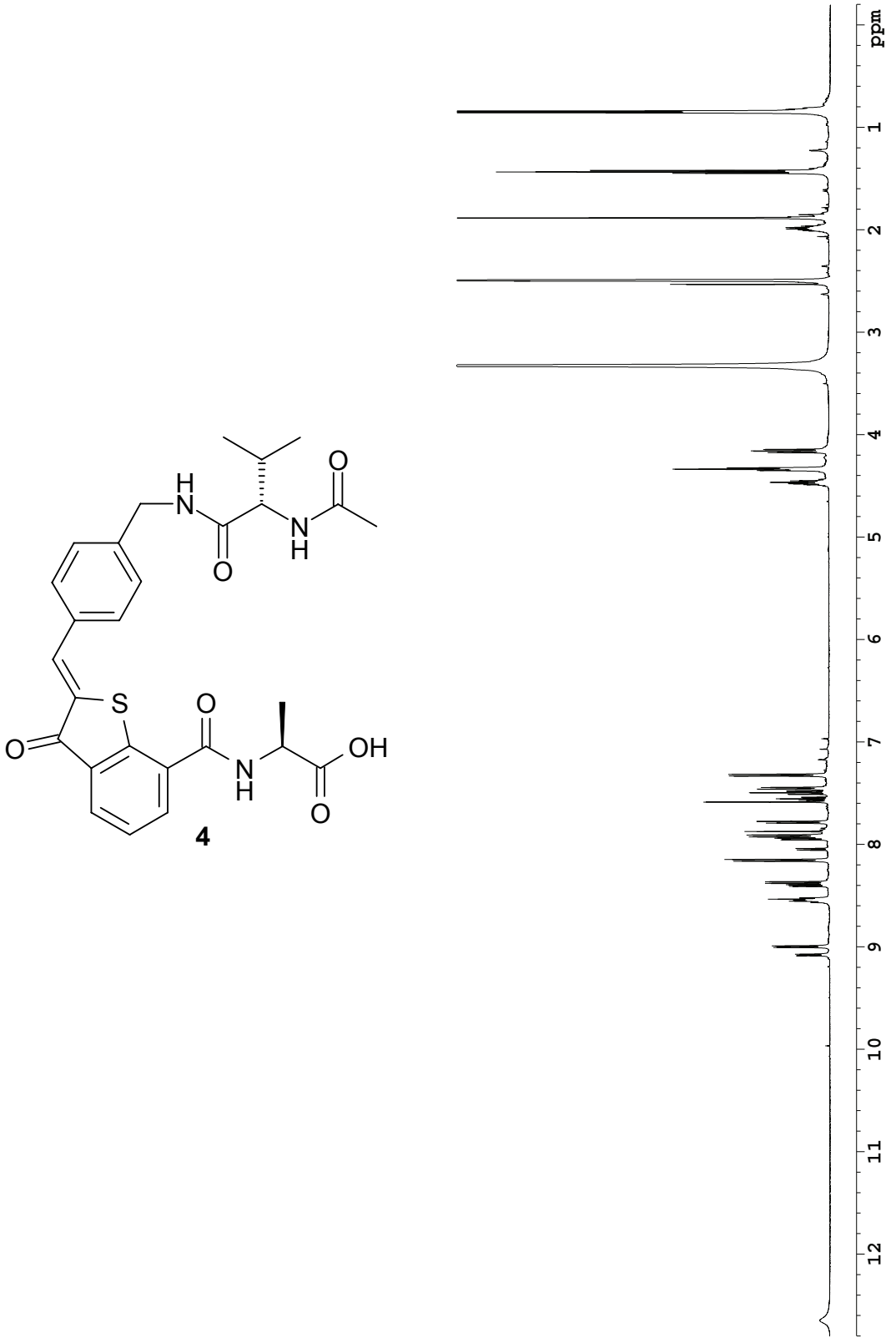

Figure S 7: ^{1}H NMR spectrum of compound photostationary mixture of **E-4** and **Z-4** (499.9 MHz, DMSO-d_6 solution, 25°C).

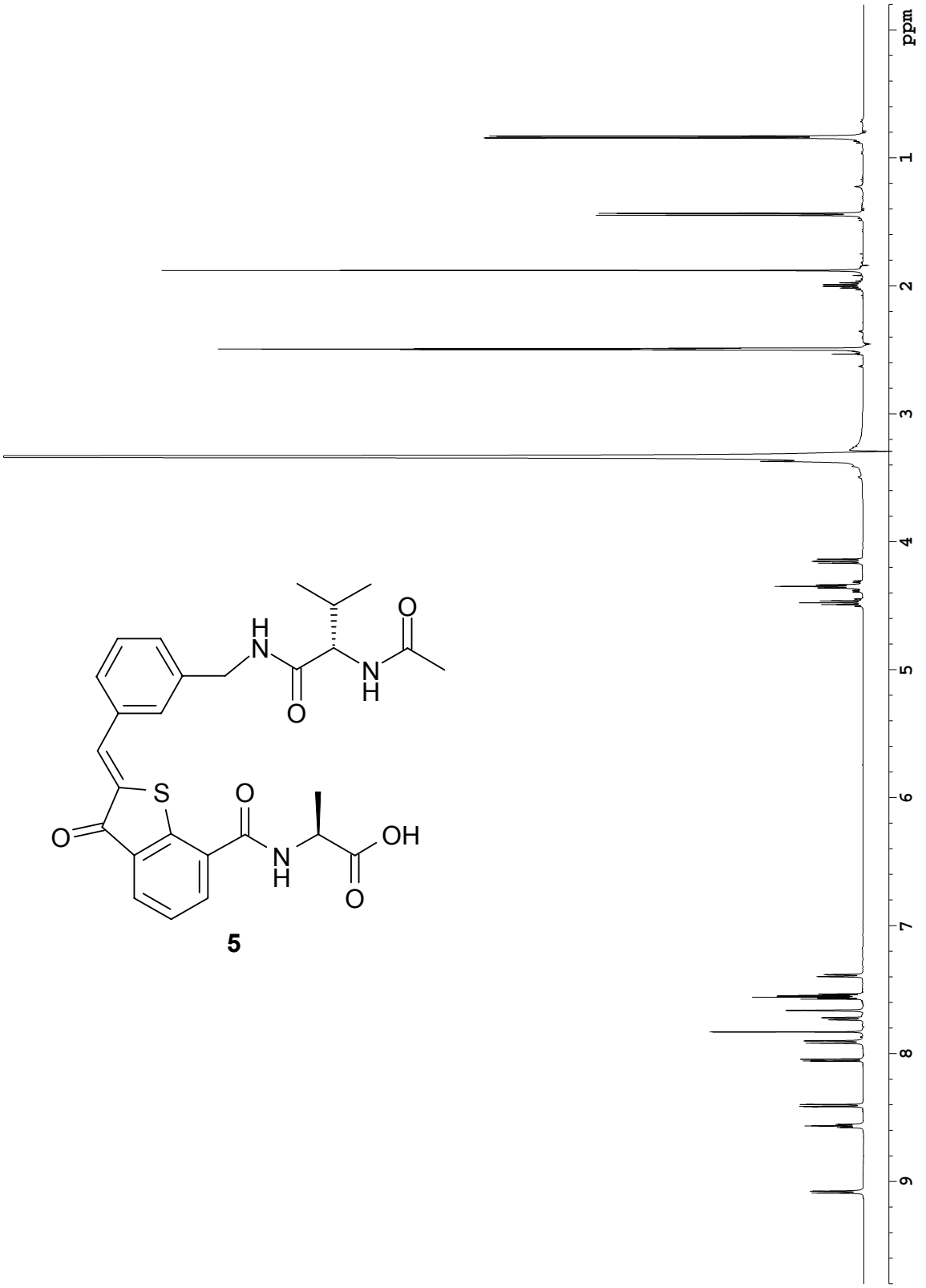

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Figure S 8: ^{1}H NMR spectrum of compound **Z-5** (499.9 MHz, DMSO-d_6 solution, 25°C).

Figure S 9: ^{1}H NMR spectrum of compound photostationary mixture of **E-5** and **Z-5** (499.9 MHz, DMSO-d_6 solution, 25°C).

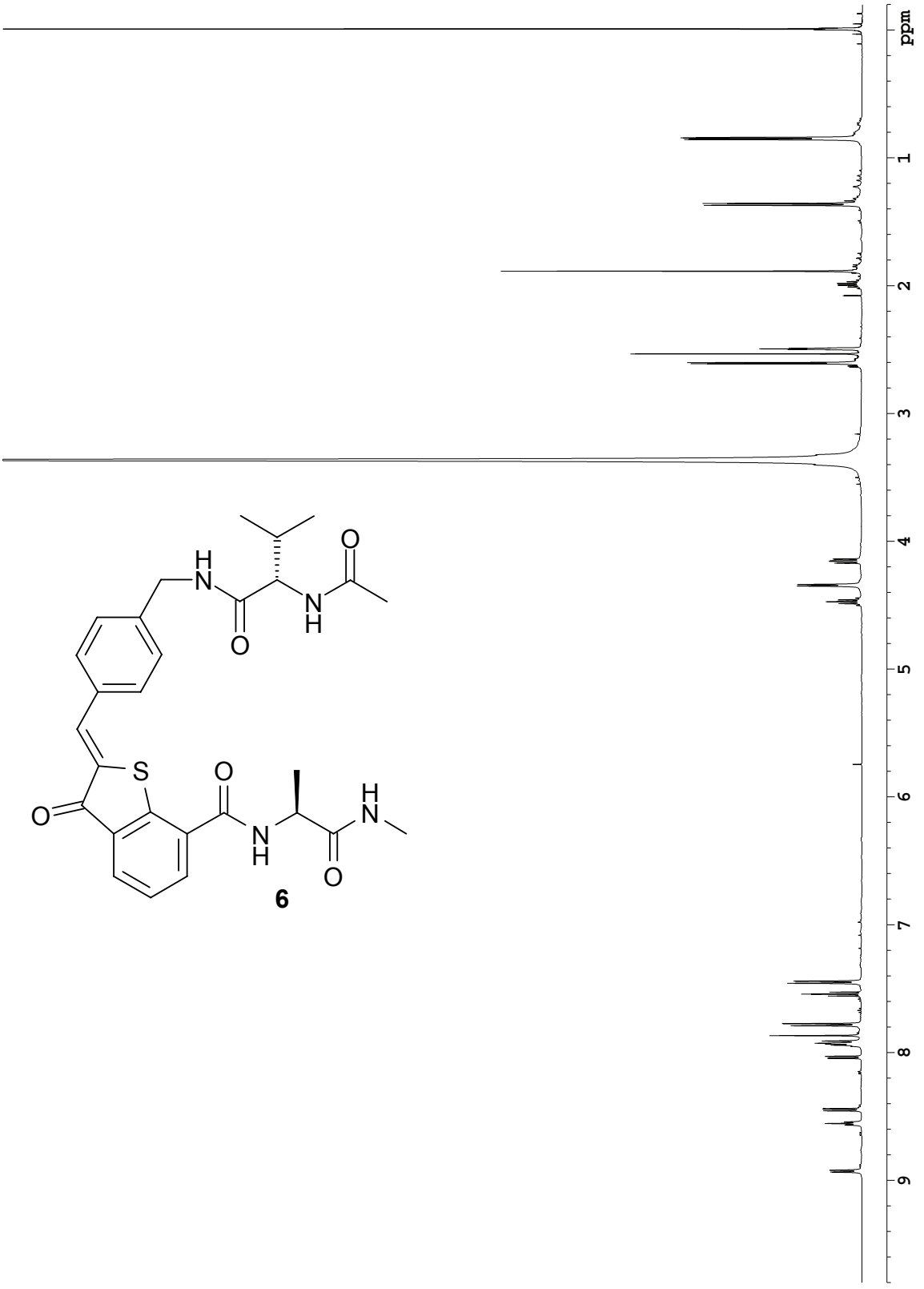

Figure S 10: ^{1}H NMR spectrum of compound **Z-6** (499.9 MHz, DMSO-d_6 solution, 25°C).

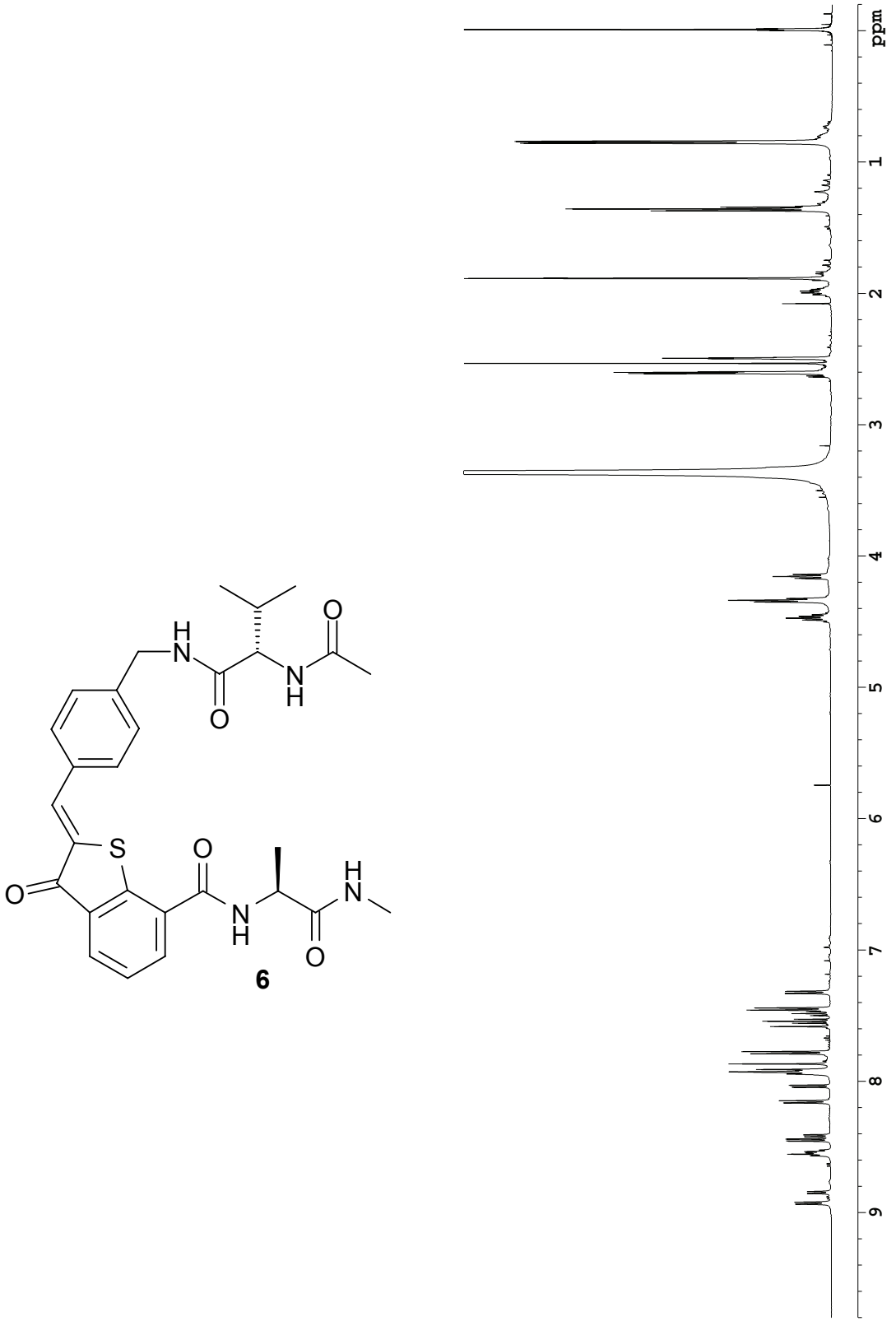

Figure S 11: ^{1}H NMR spectrum of compound photostationary mixture of **E-6** and **Z-6** (499.9 MHz, DMSO-d_6 solution, 25°C).

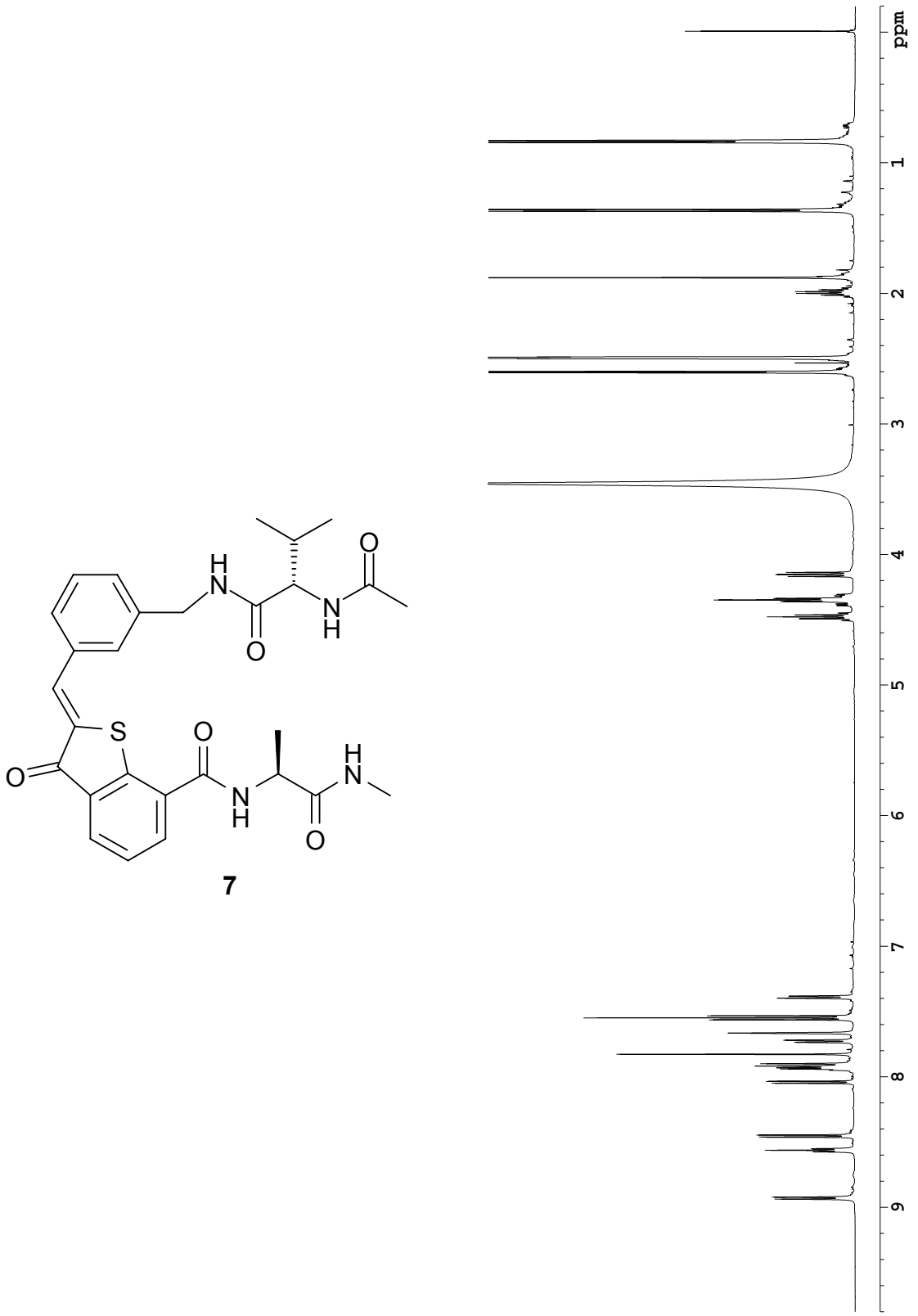

Figure S 12: ^{1}H NMR spectrum of compound **Z-7** (499.9 MHz, DMSO-d_6 solution, 25°C).

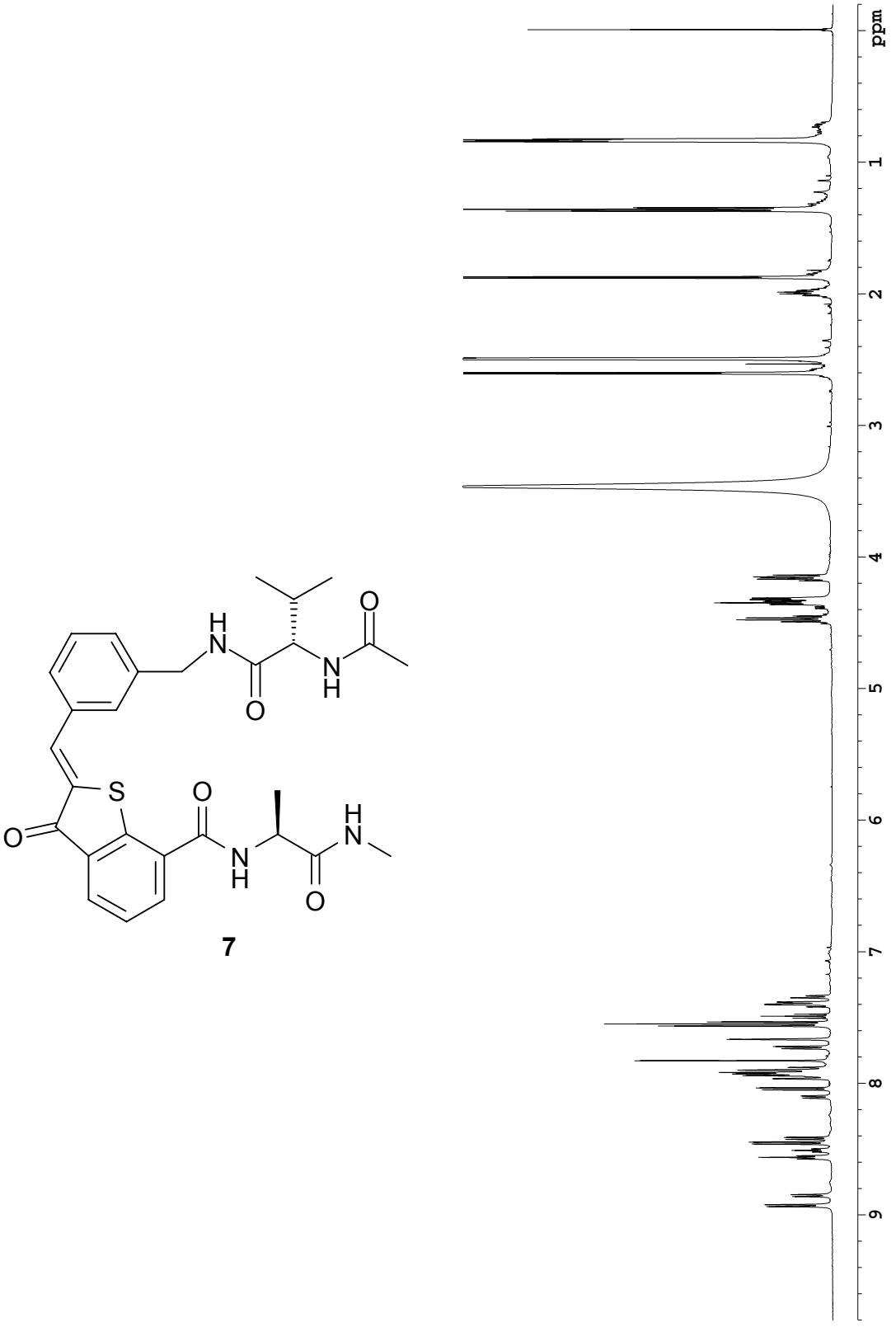

Figure S 13: ^{1}H NMR spectrum of compound photostationary mixture of **E-7** and **Z-7** (499.9 MHz, DMSO-d_6 solution, 25°C).

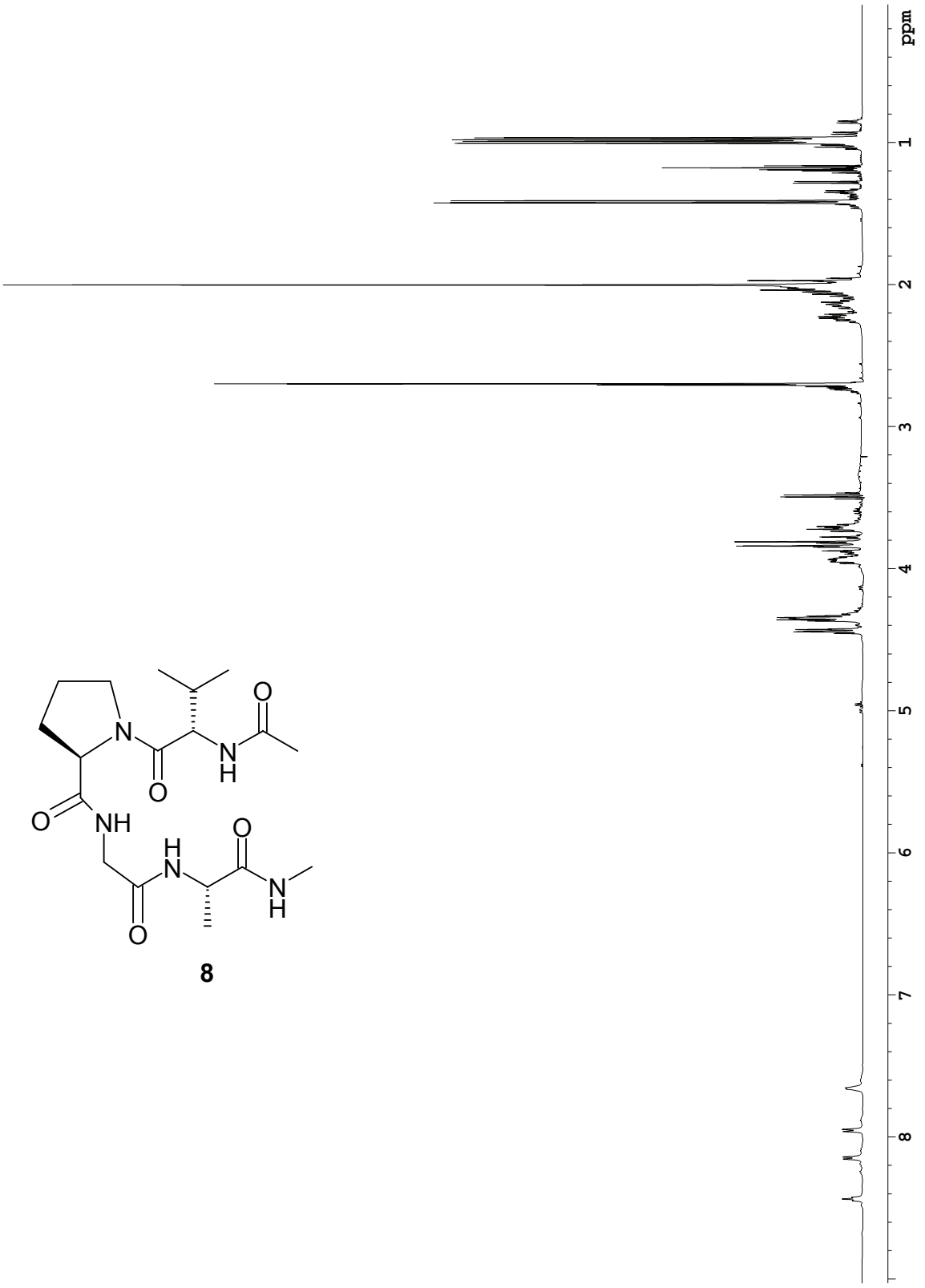

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Figure S 14: ^{1}H NMR spectrum of compound **8** (499.9 MHz, CD_3OD/CH_3OH (1:1) solution, solvent suppression used, 25°C).

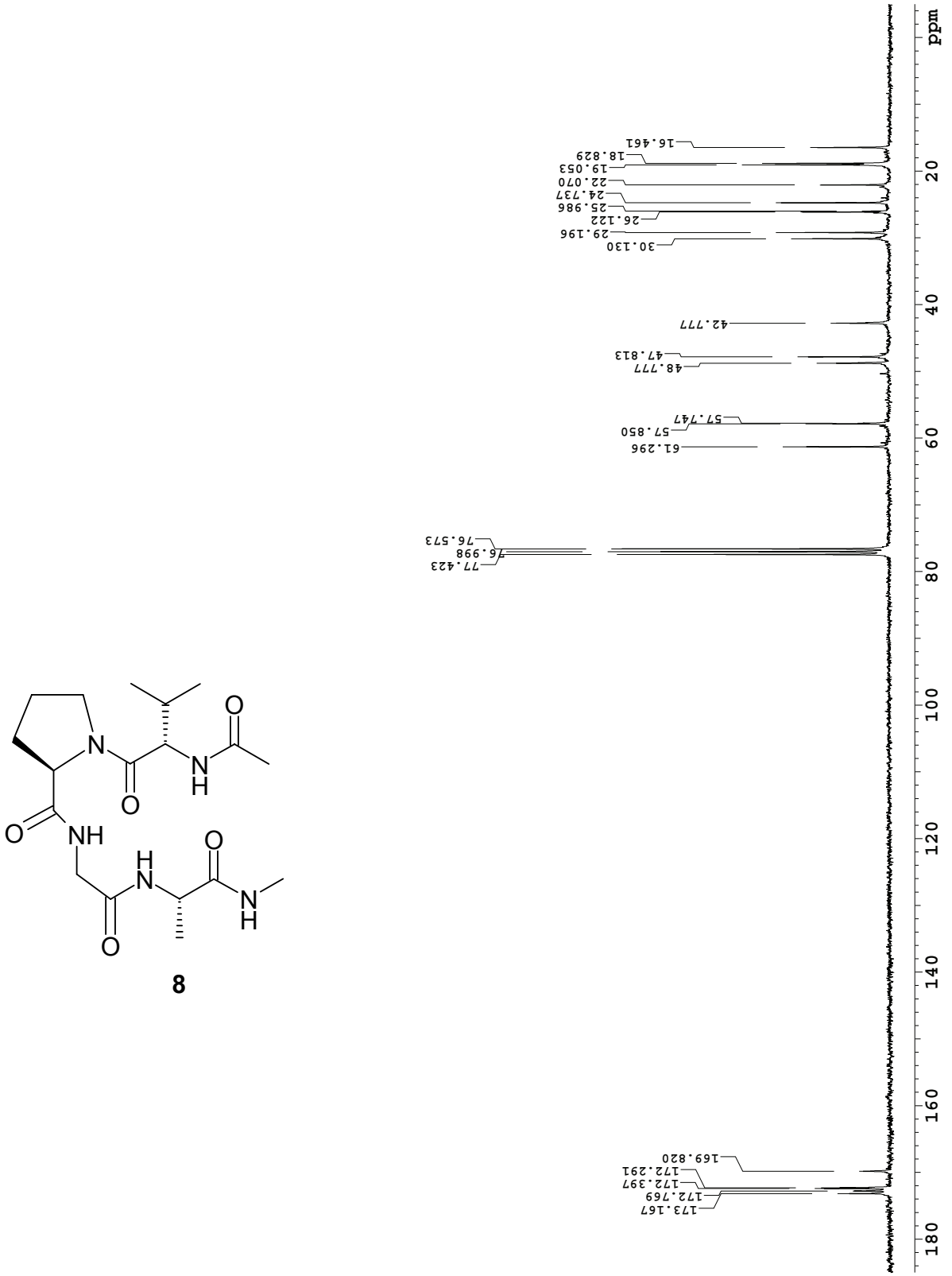

Figure S 15: ^{13}C NMR spectrum of compound **8** (75 MHz, $CDCl_3$ solution, 25°C).

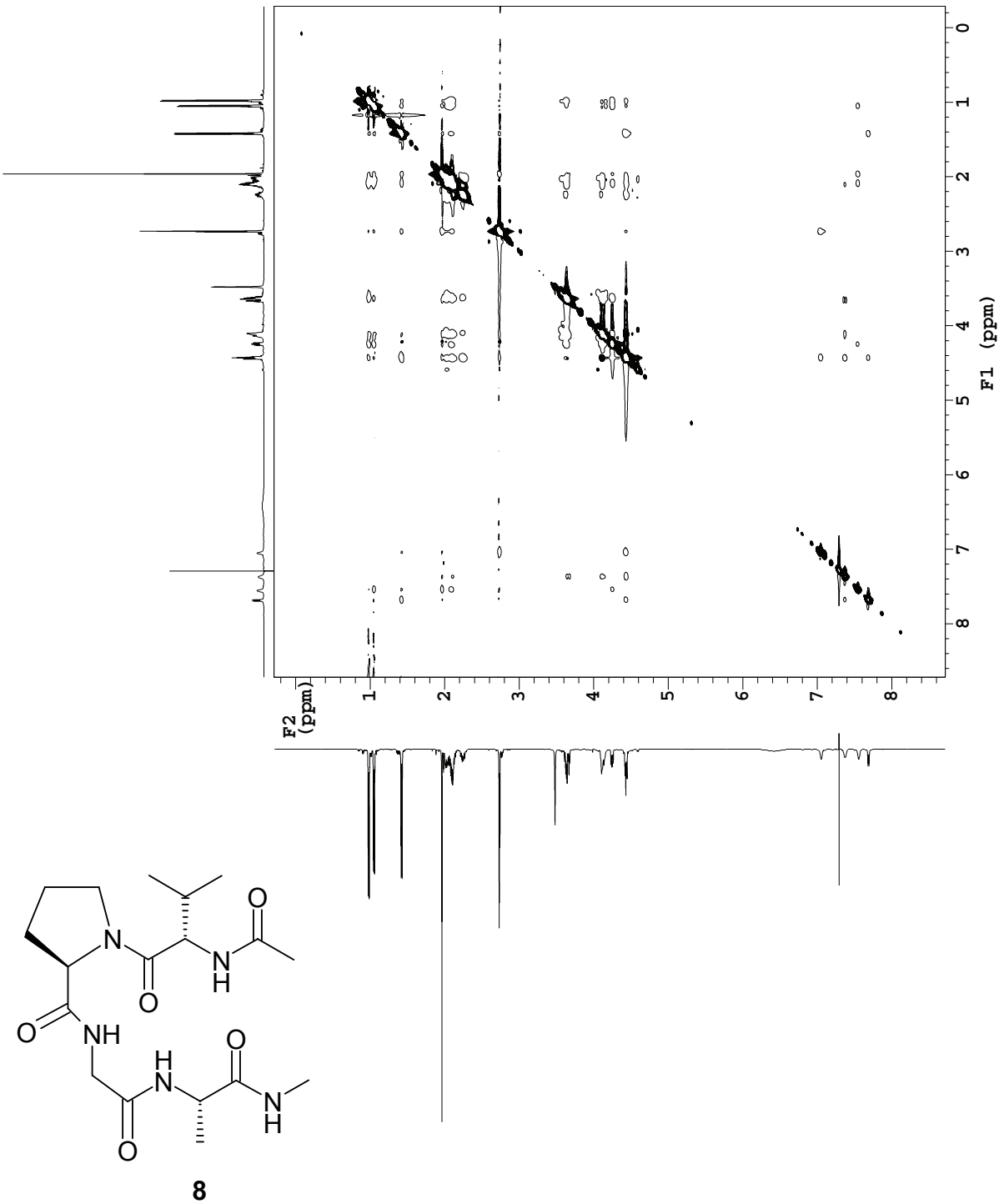

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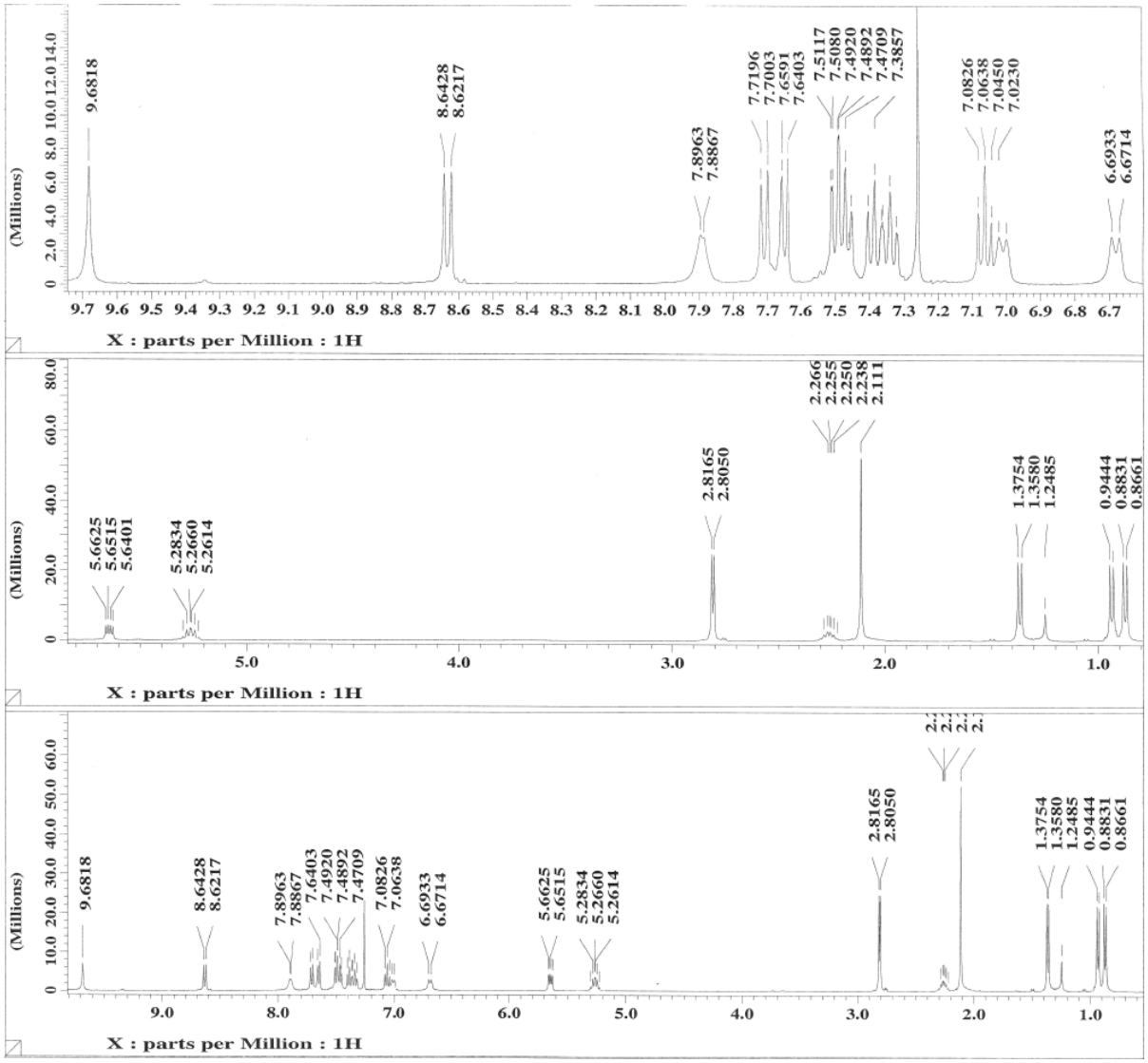
Figure S 16: ROESY spectrum of compound **8** (499.9 MHz, $CDCl_3$ solution, 25°C).



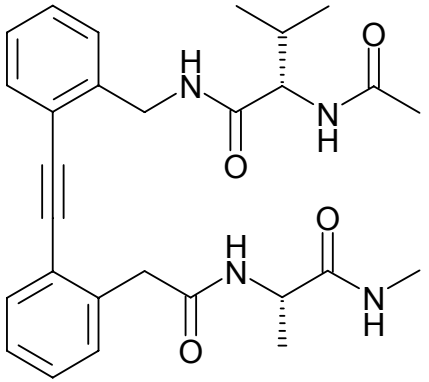


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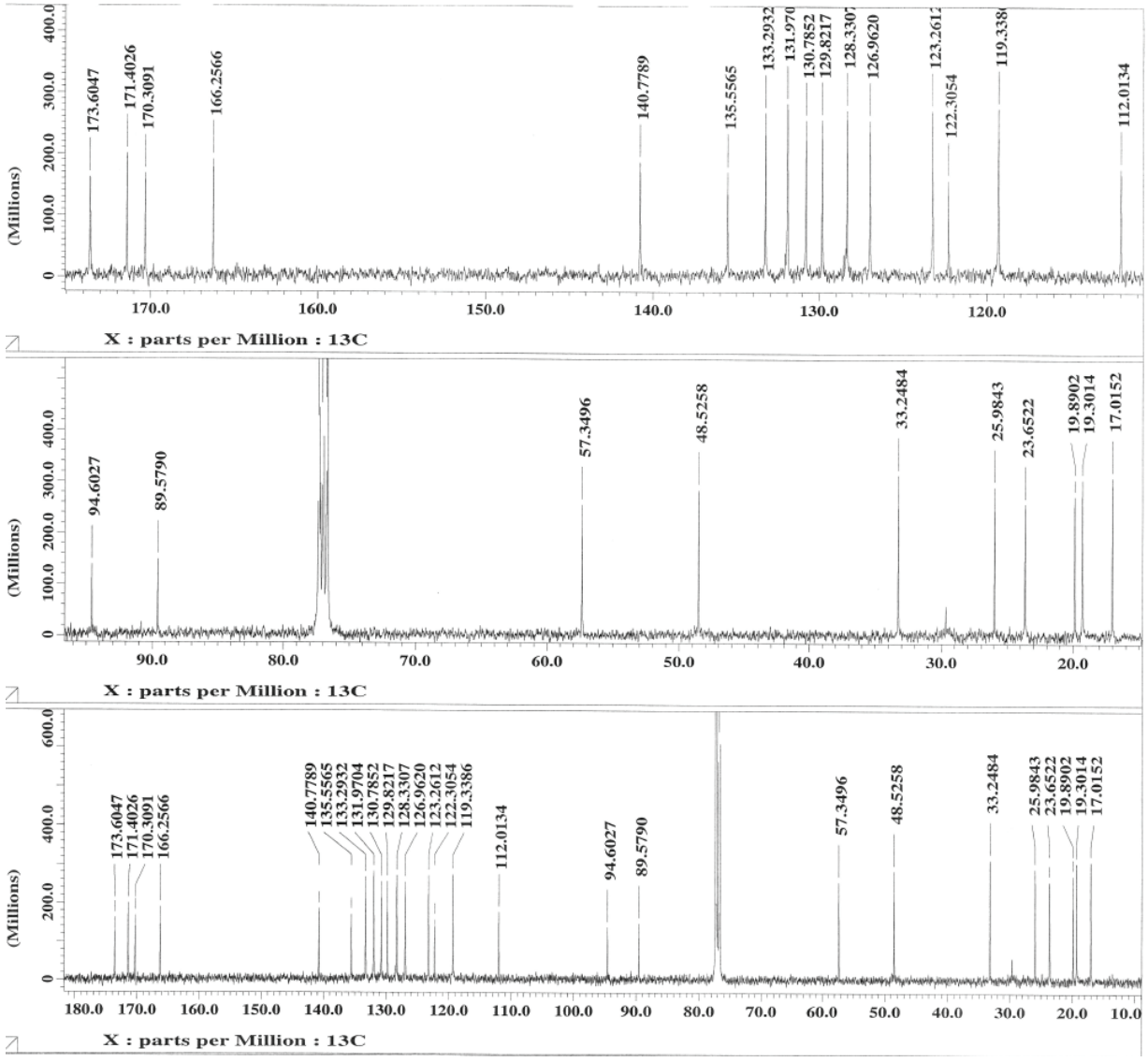
Figure S 17: ^{1}H NMR spectrum of compound **10** (399.8 MHz, DMSO-d_6 solution, 25°C).



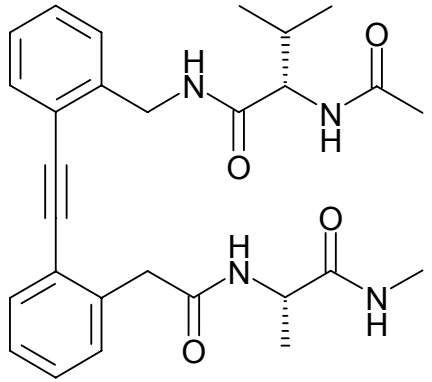


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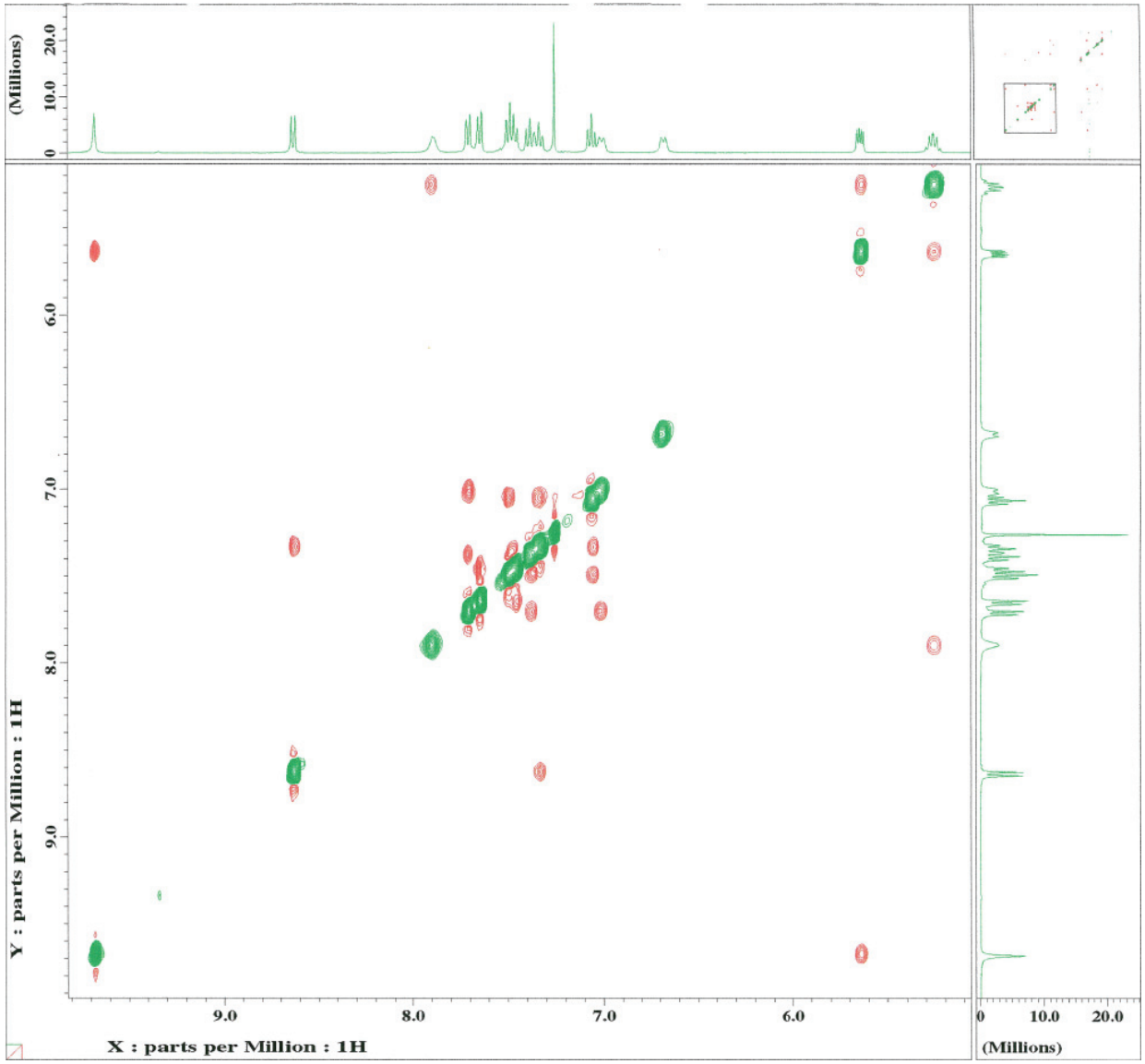
Figure S 18: ^{13}C NMR spectrum of compound **10** (75 MHz, DMSO-d_6 solution, 25°C).



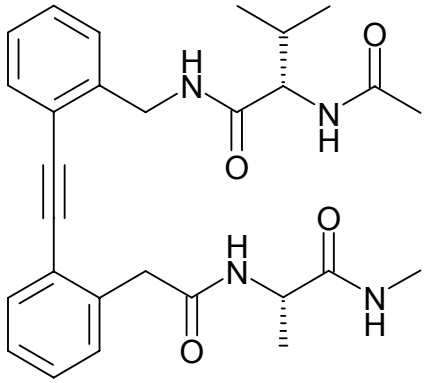


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Figure S 19: NOESY spectrum of compound **10** (399.8 MHz, DMSO-d_6 solution, 25°C).

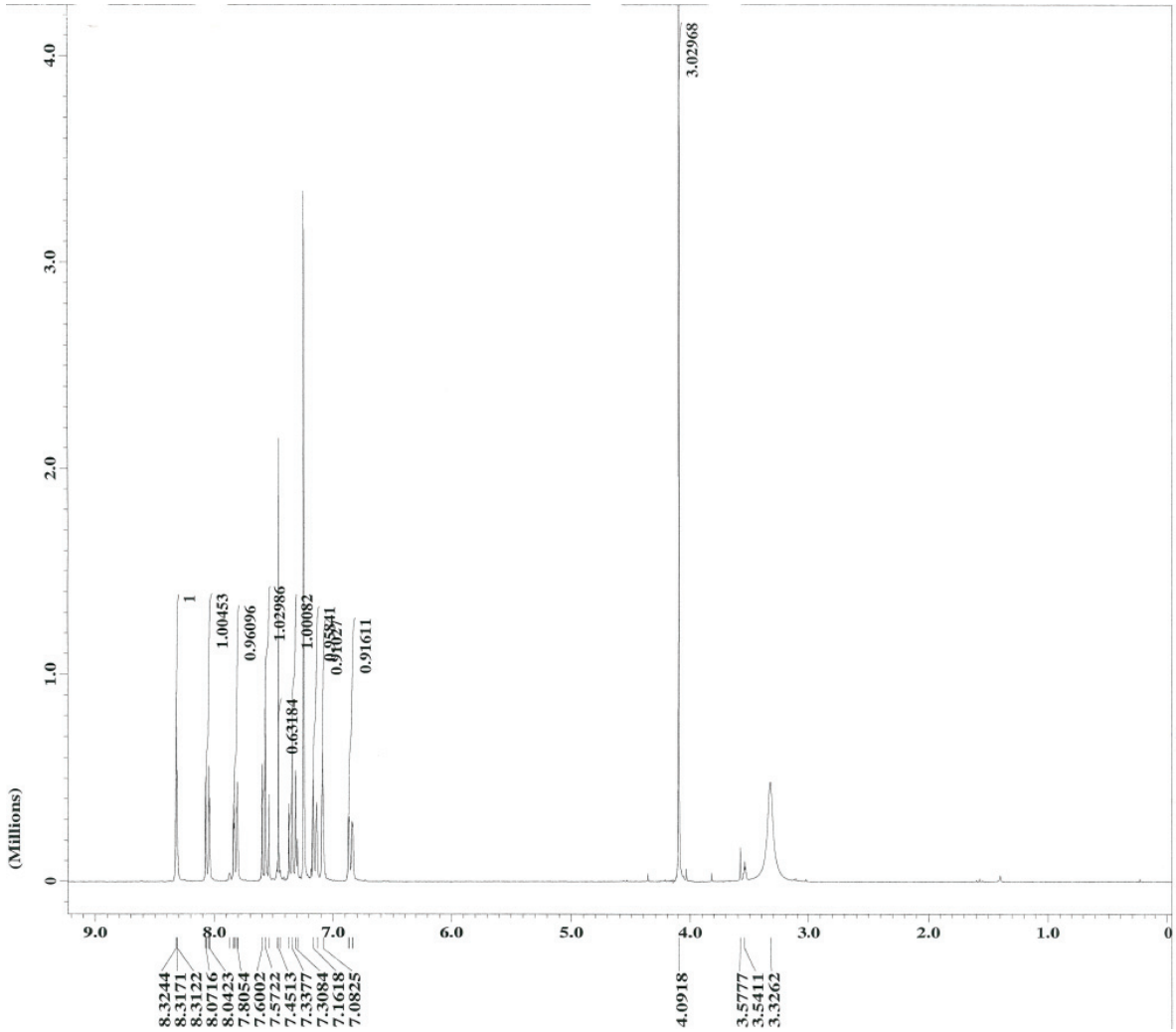

Figure S 20: ^{1}H NMR spectrum of compound **12** (270.2 MHz, $CDCl_3$ solution, 25°C).

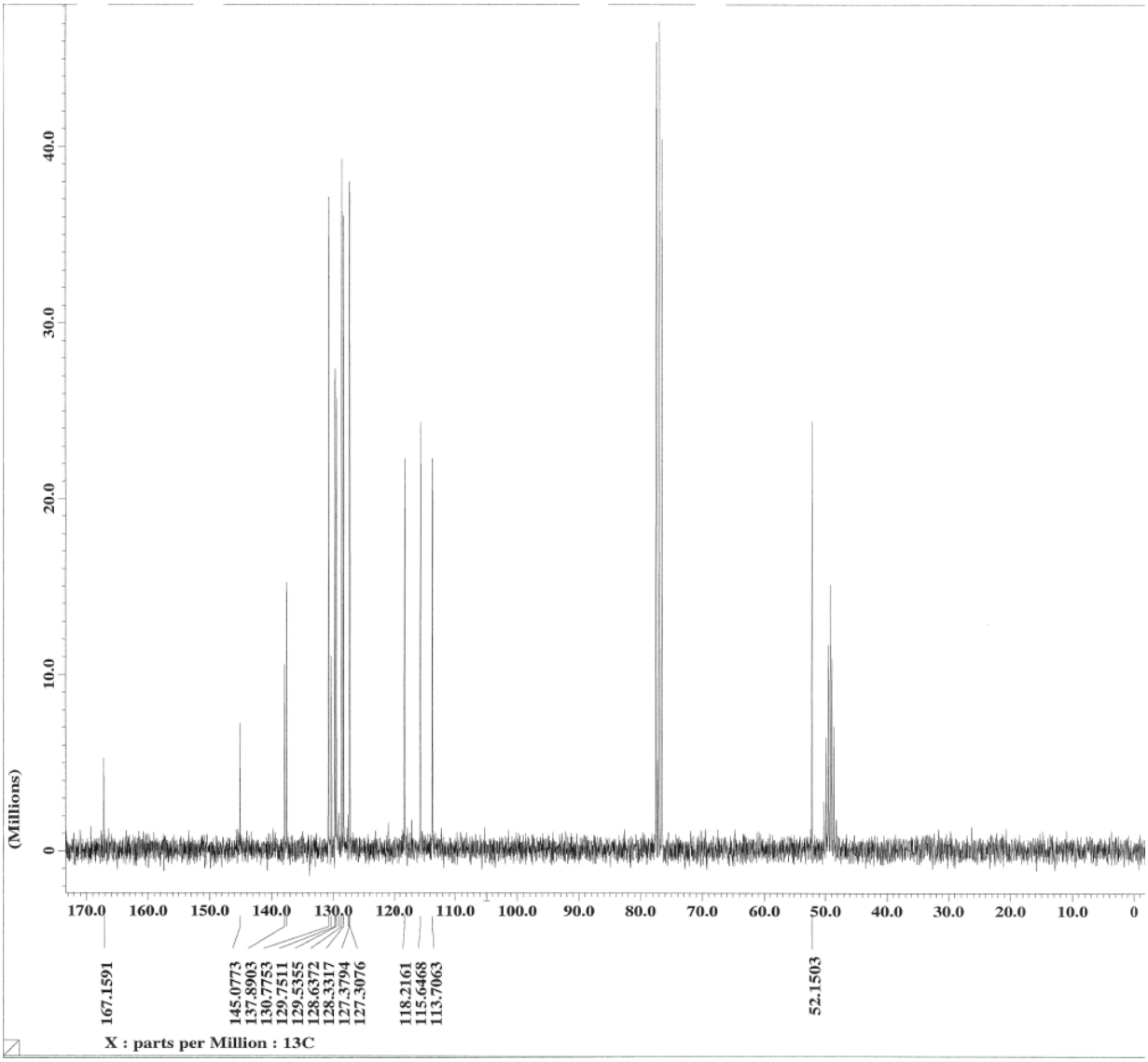

Figure S 21: ^{13}C NMR spectrum of compound **12** (67.9 MHz, $CDCl_3$ solution, 25°C).

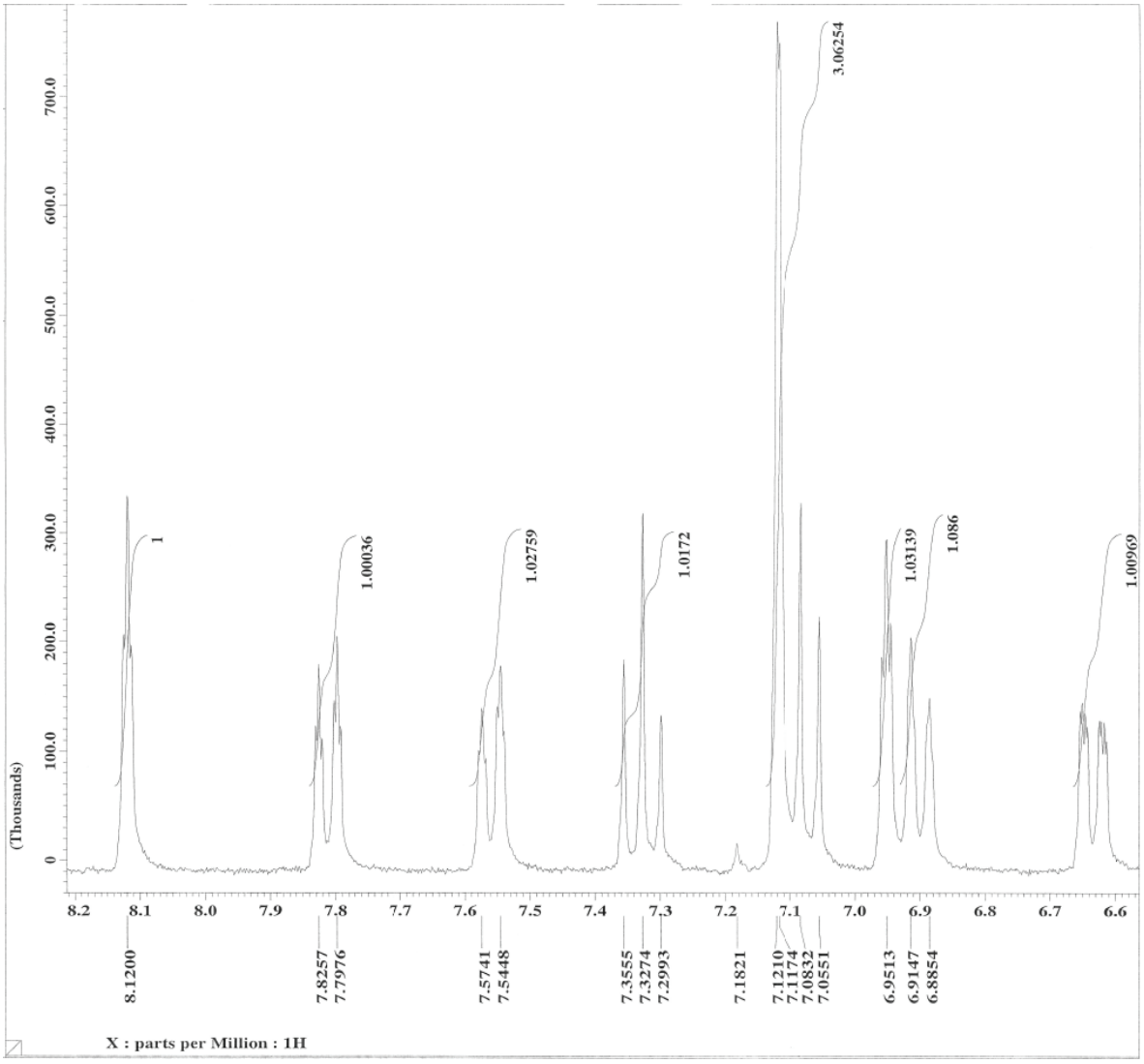

Figure S 22: ^{1}H NMR spectrum of compound **13** (399.9 MHz, CD_3OD solution, 25°C).

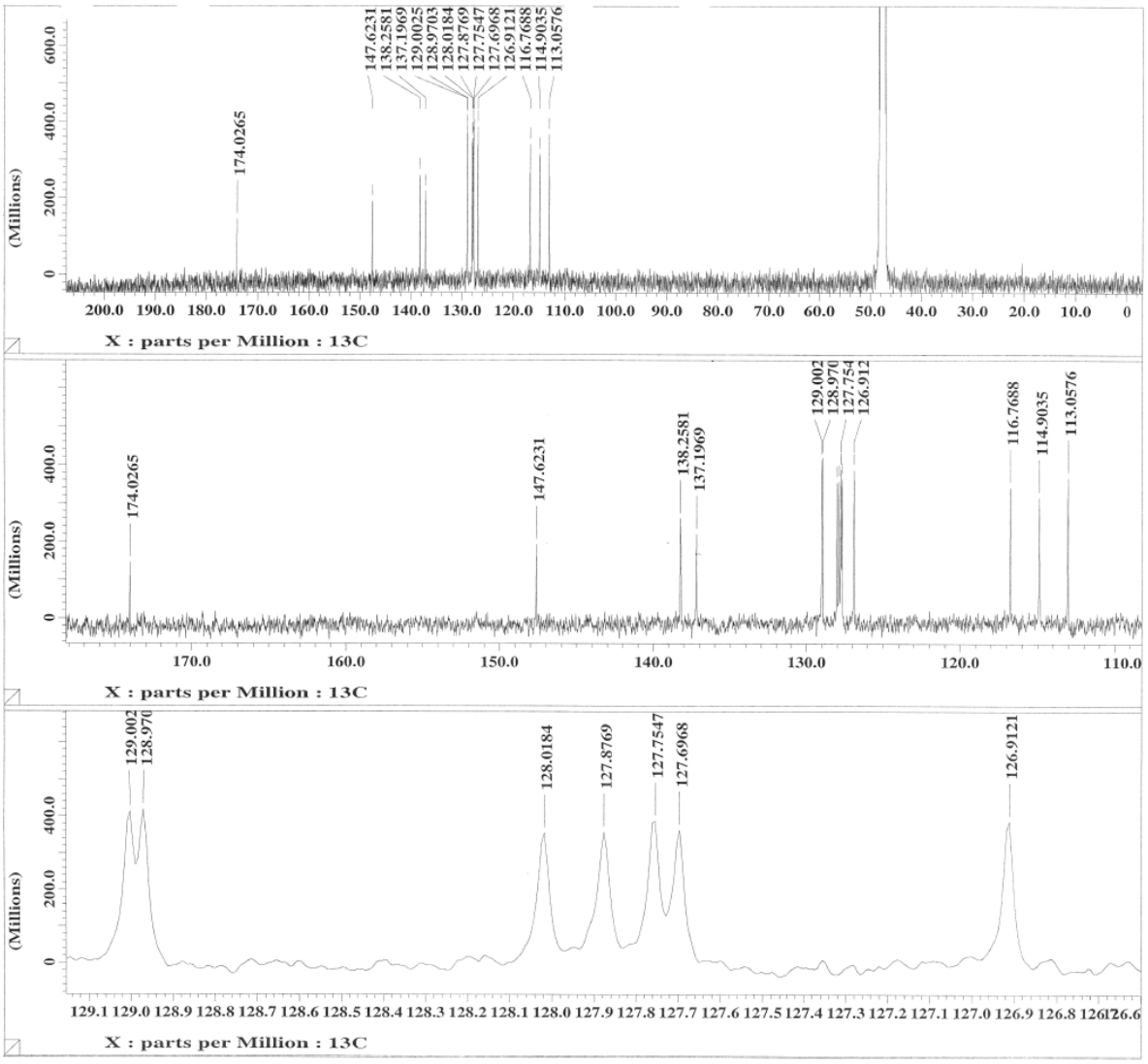

Figure S 23: ^{13}C NMR spectrum of compound **13** (100.5 MHz, CD_3OD solution, 25°C).

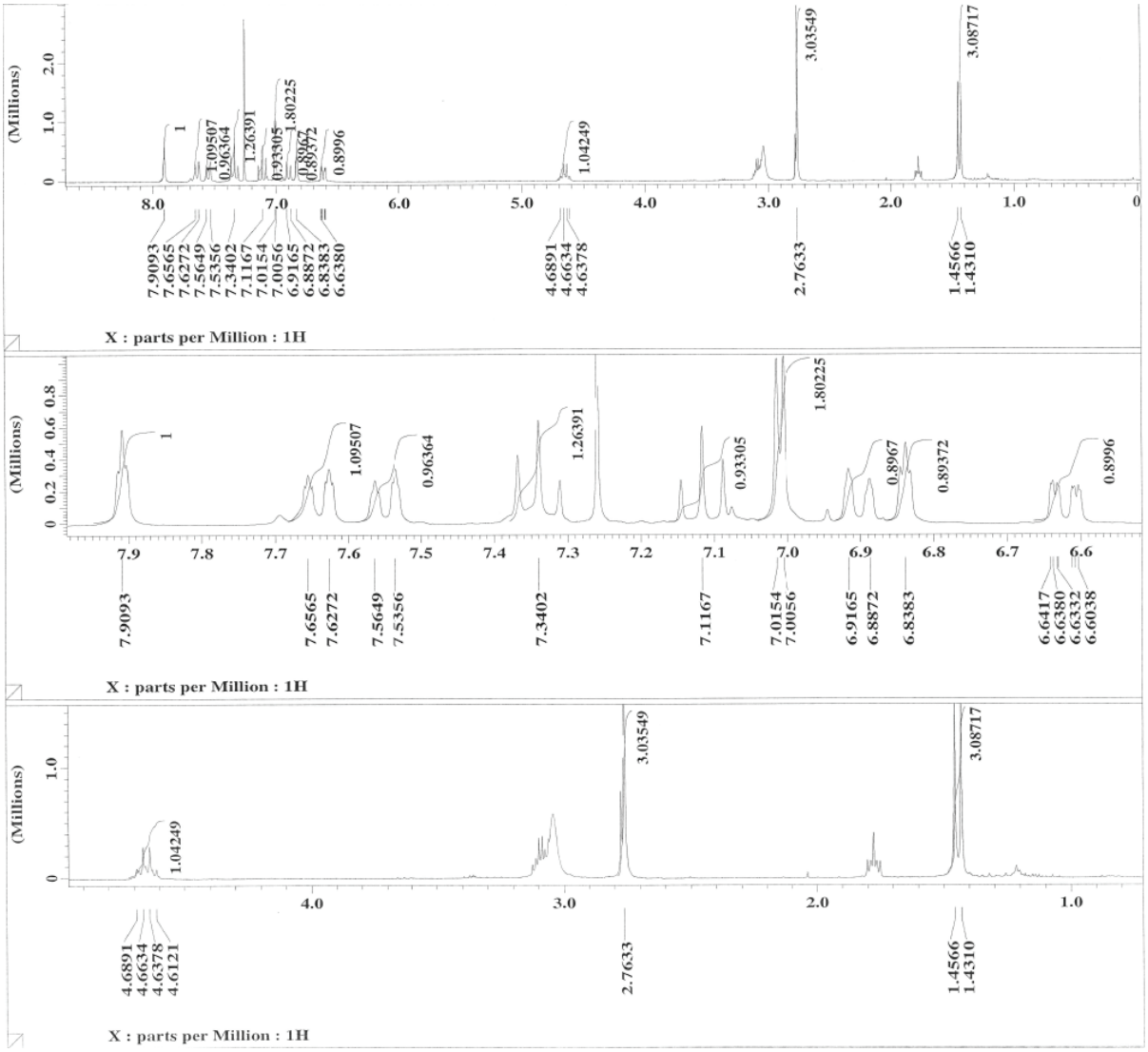

Figure S 24: ^{1}H NMR spectrum of compound **14** (270.2 MHz, $CDCl_3$ solution, 25°C).

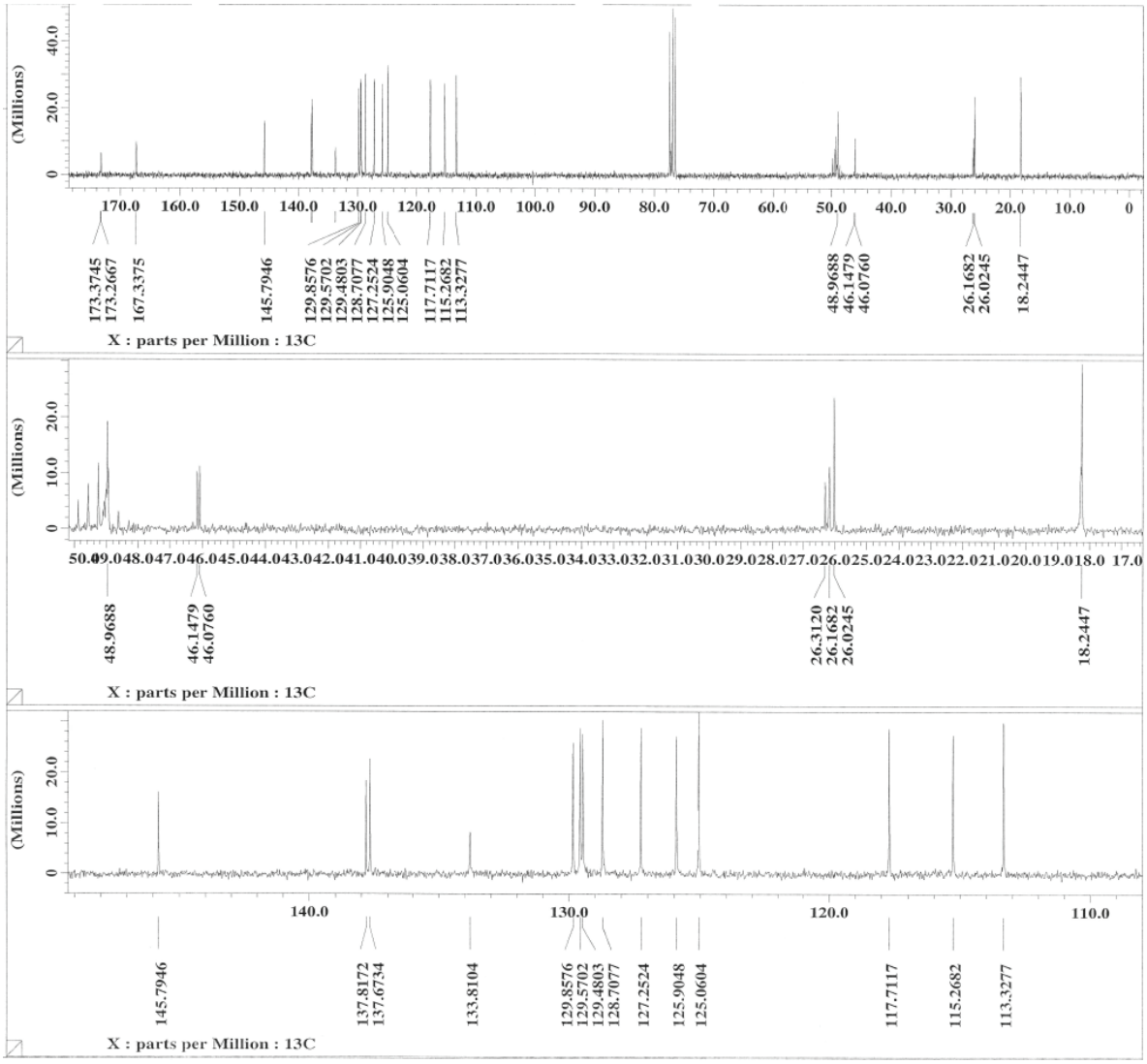

Figure S 25: ^{13}C NMR spectrum of compound **14** (67.9 MHz, $CDCl_3$ solution, 25°C).

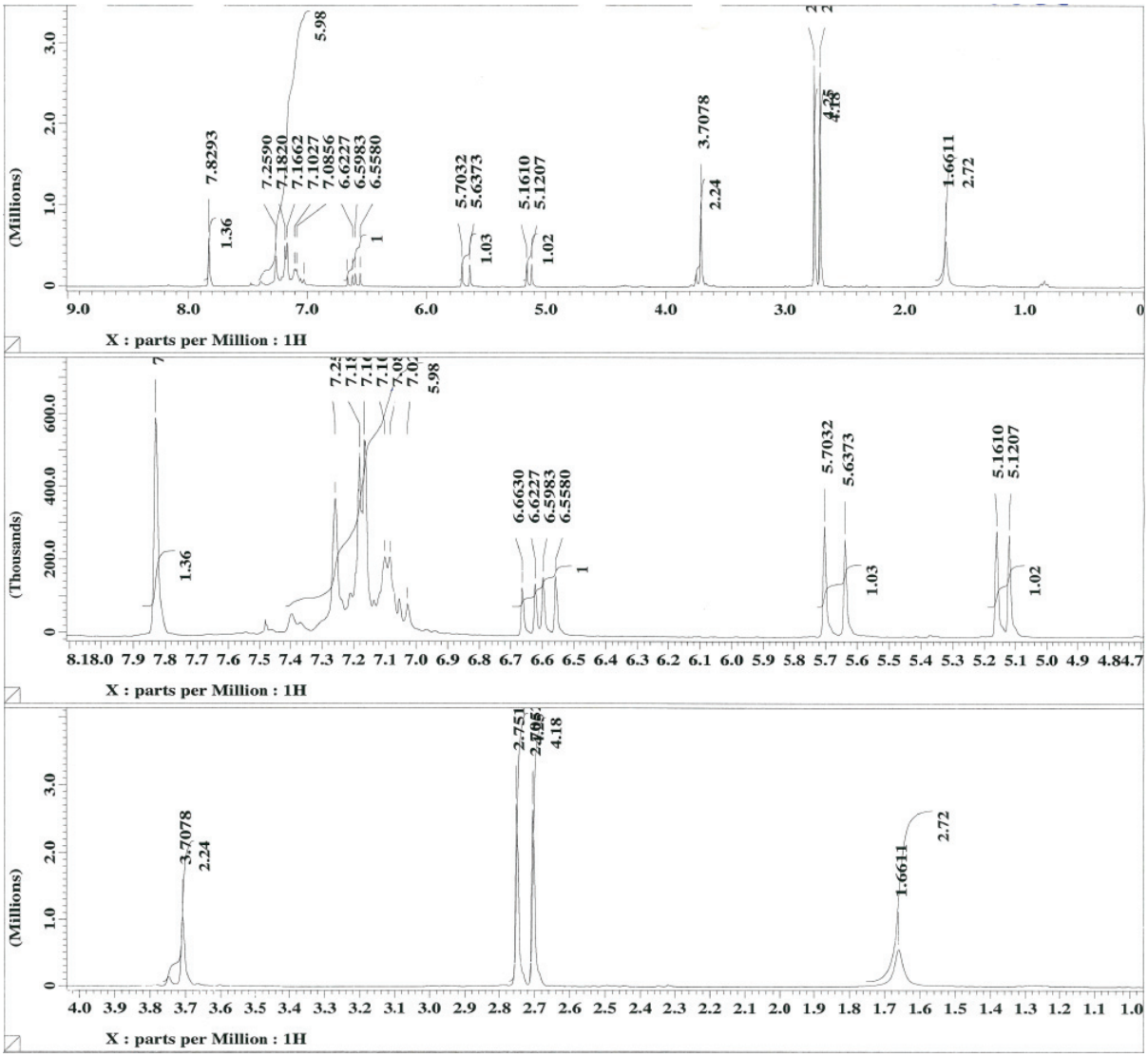

Figure S 26: ^{1}H NMR spectrum of compound **16** (270.2 MHz, $CDCl_3$ solution, 25°C).

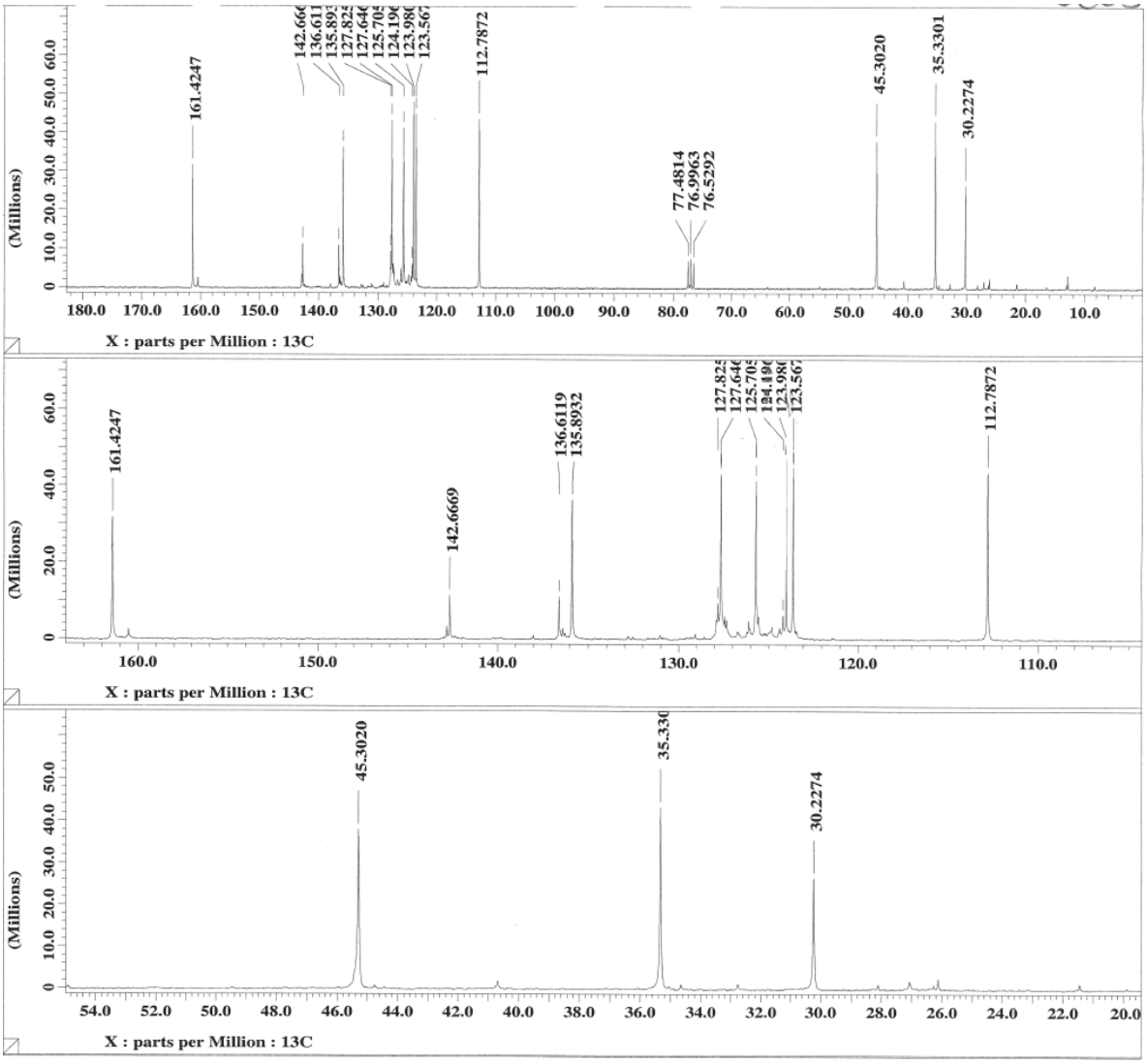

Figure S 27: ^{13}C NMR spectrum of compound **16** (67.9 MHz, $CDCl_3$ solution, 25°C).

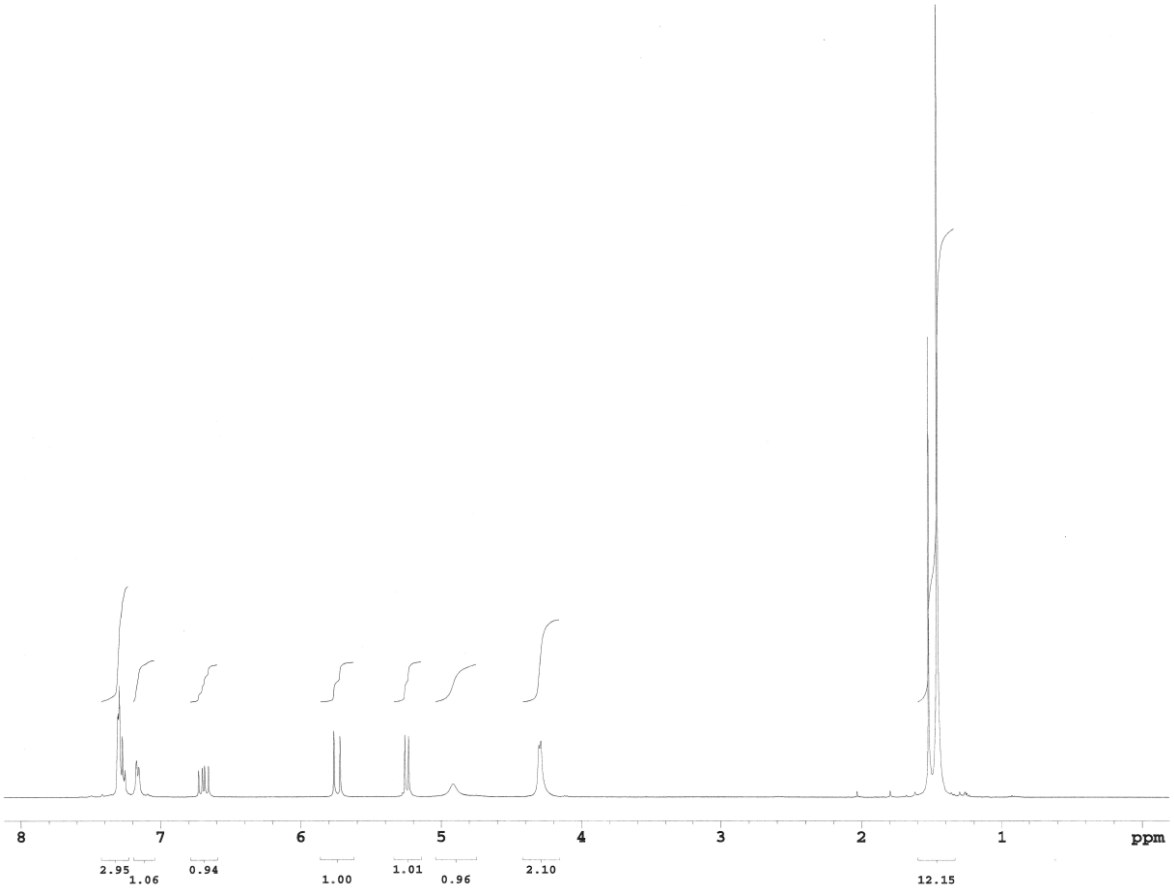

Figure S 28: ^{1}H NMR spectrum of compound **17** (399.9 MHz, $CDCl_3$ solution, 25°C).

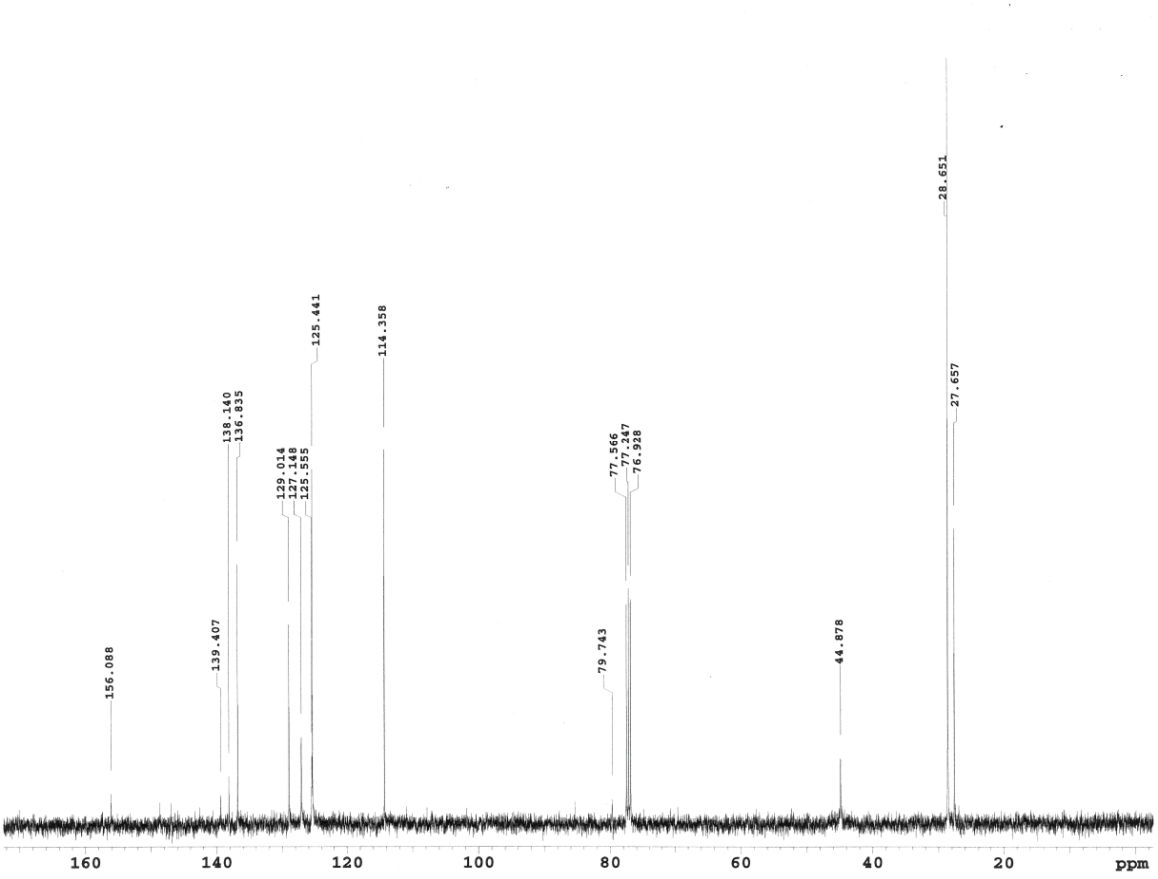

Figure S 29: ^{13}C NMR spectrum of compound **17** (100.6 MHz, $CDCl_3$ solution, 25°C).

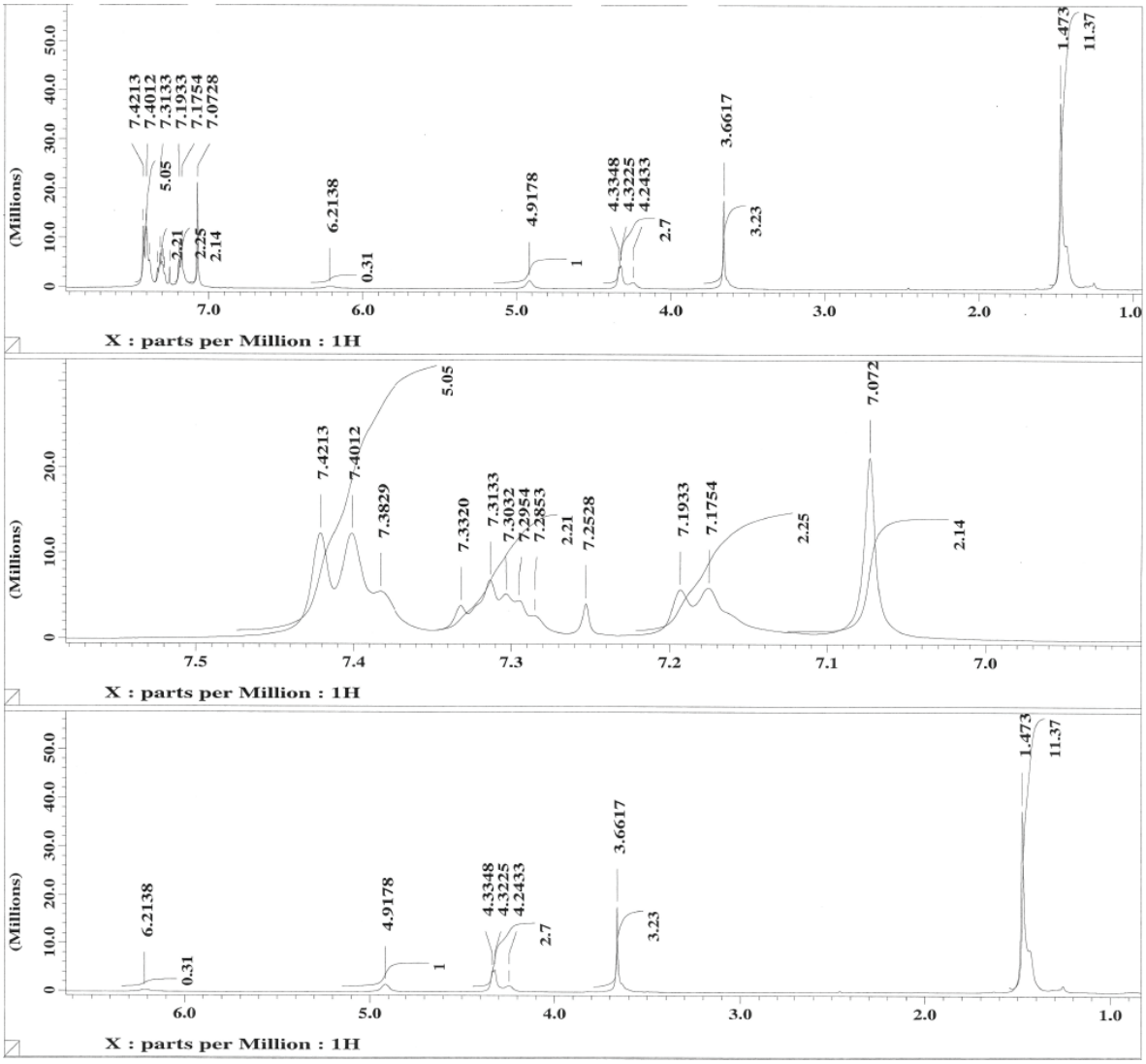

Figure S 30: ^{1}H NMR spectrum of compound **19** (399.8 MHz, $CDCl_3$ solution, 25°C).

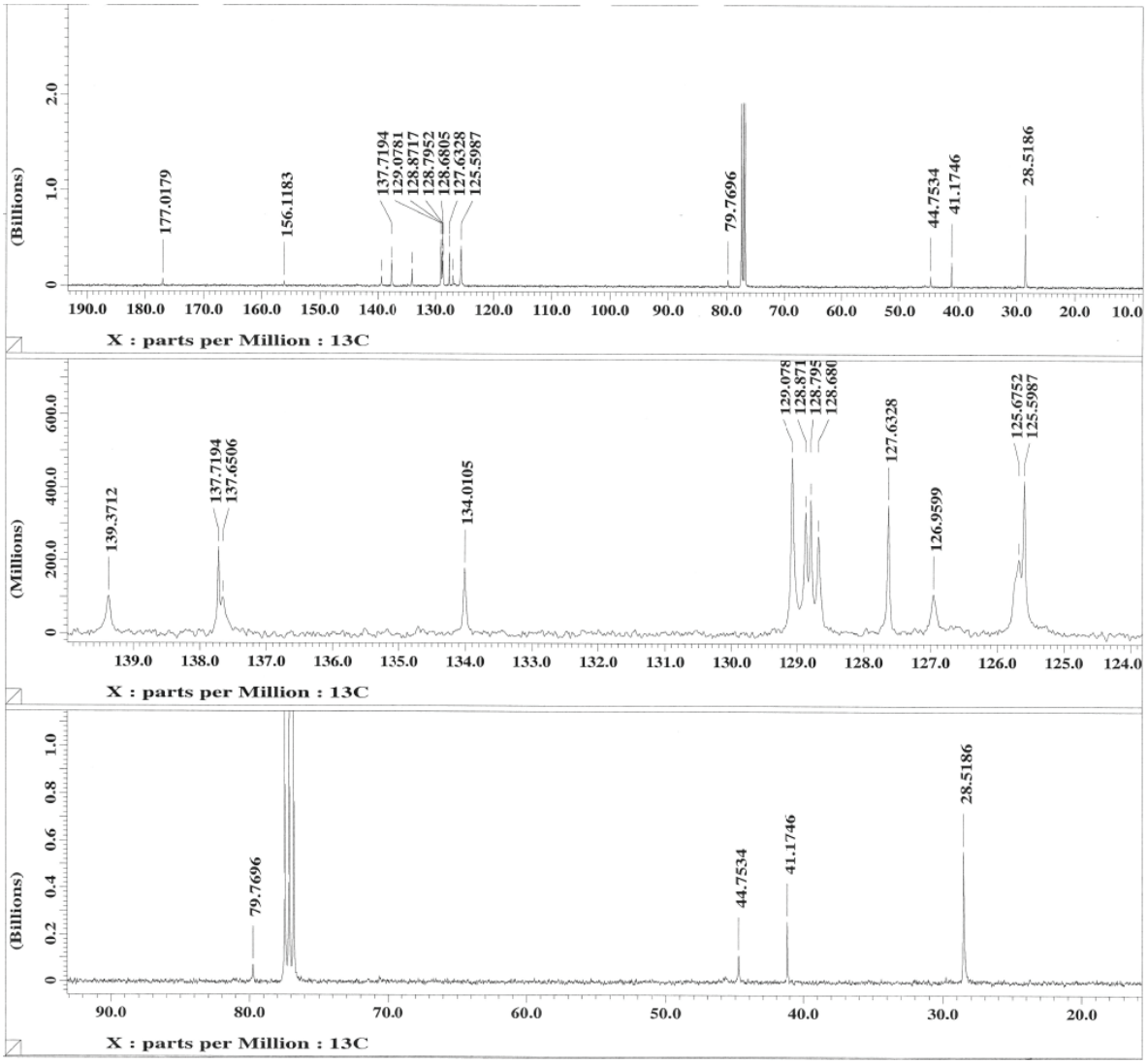

Figure S 31: ^{13}C NMR spectrum of compound **19** (100.5 MHz, $CDCl_3$ solution, 25°C).

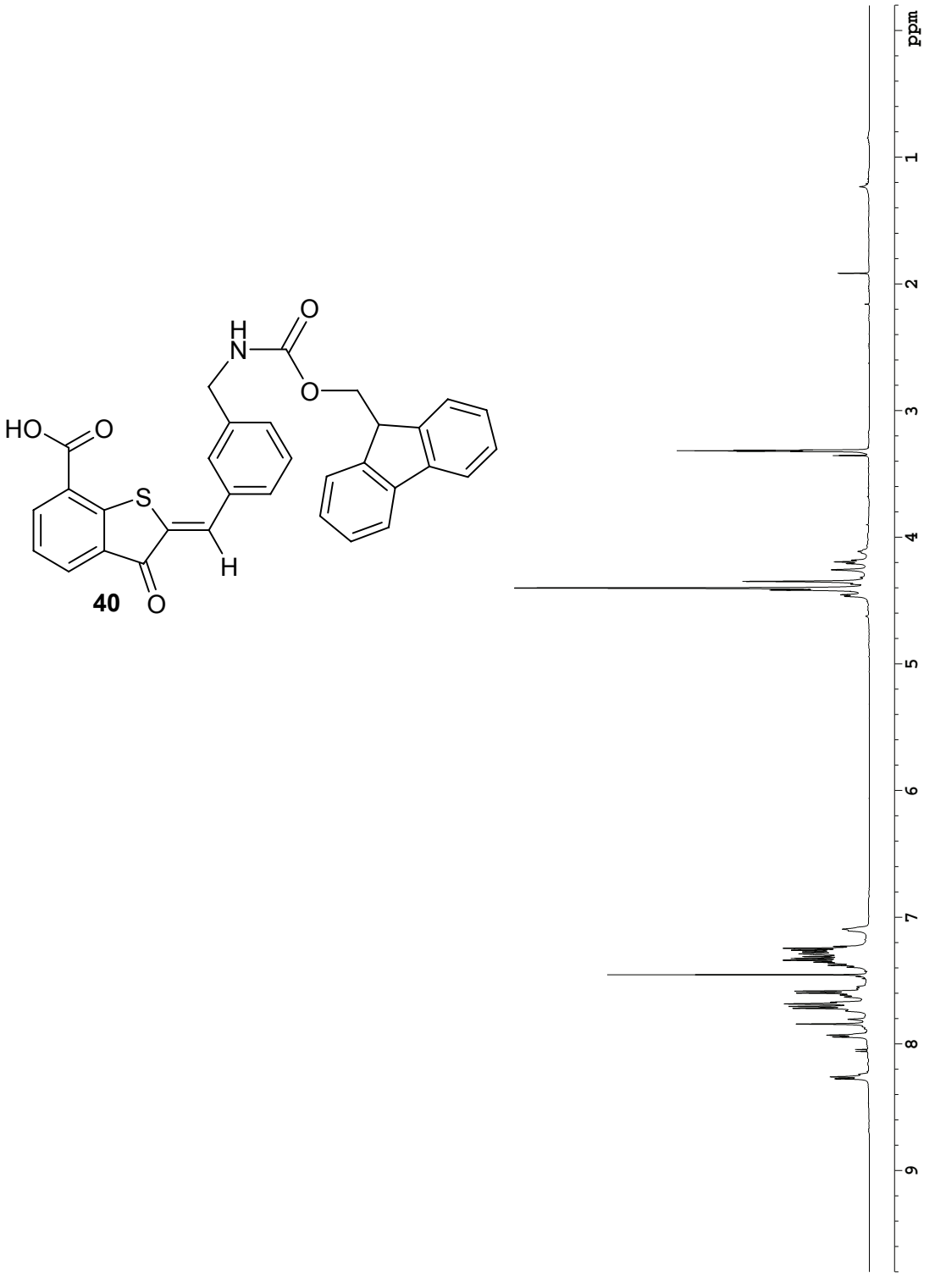

Figure S 32: ^{1}H NMR spectrum of compound **40** (499.9 MHz, $CD_3OD/CDCl_3$ (3:1) solution, 25°C).

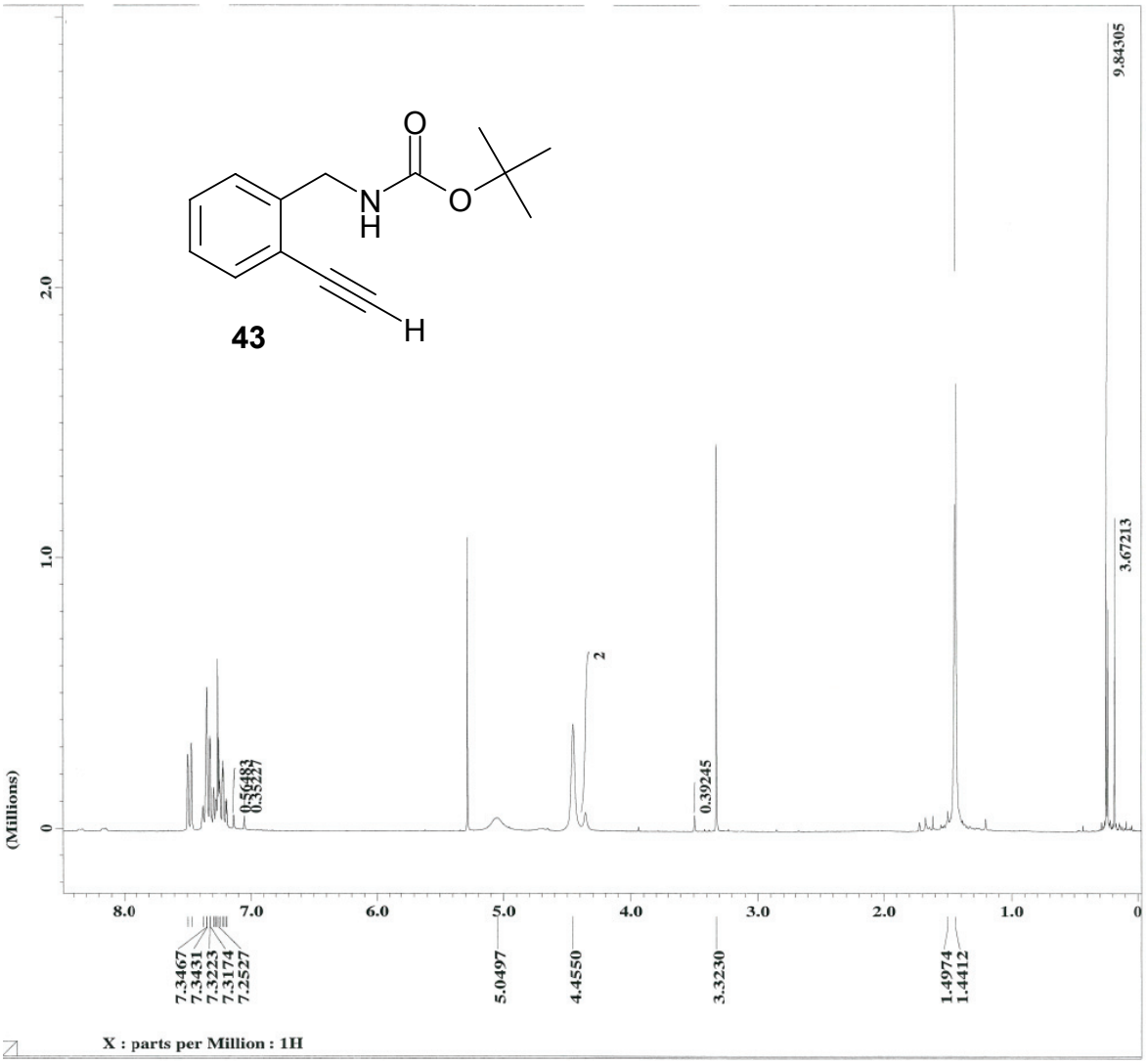

Figure S 33: ^{1}H NMR spectrum of compound **43** (270.2 MHz, $CDCl_3$ solution, 25°C).

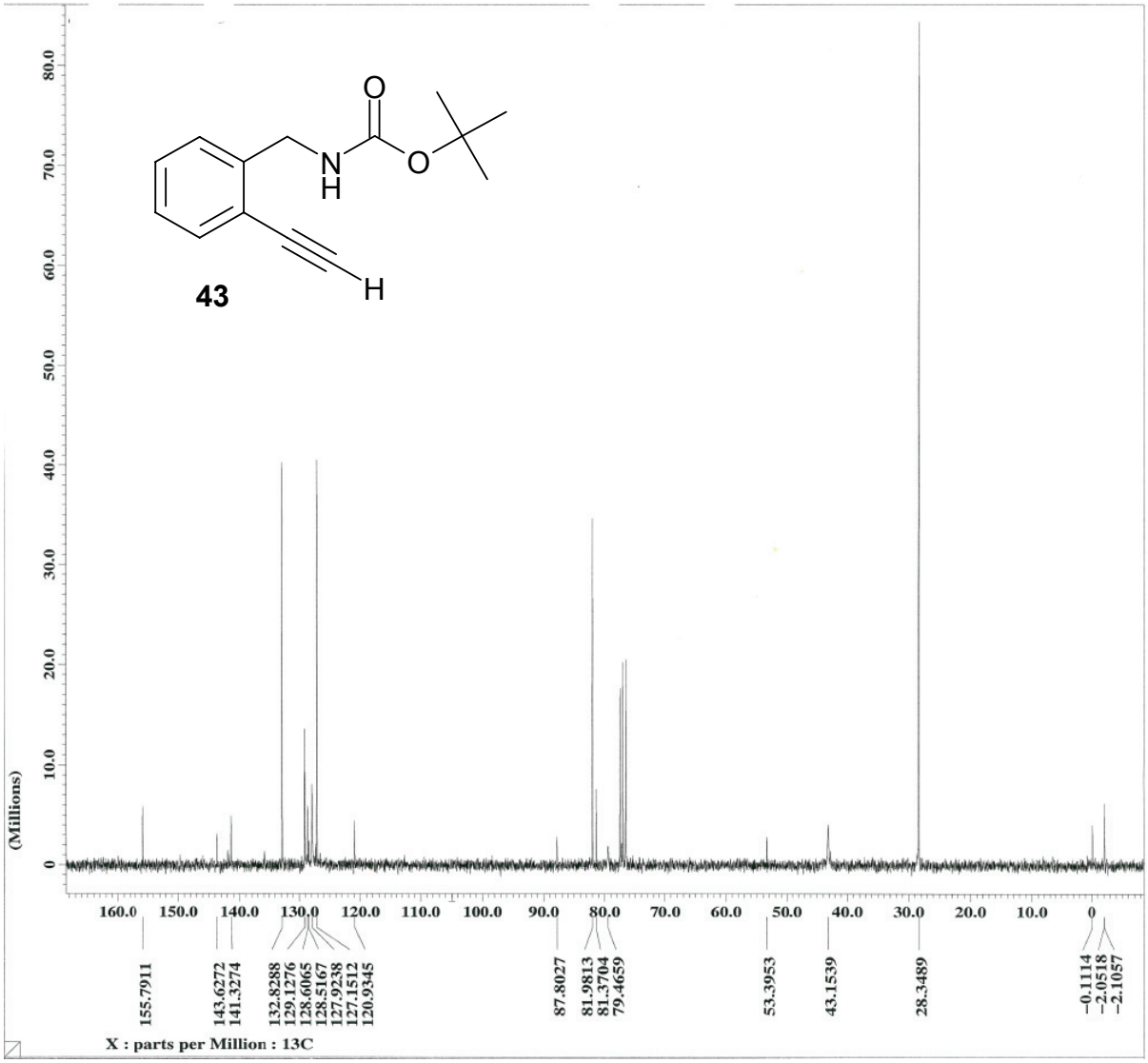

Figure S 34: ^{13}C NMR spectrum of compound **43** (67.9 MHz, $CDCl_3$ solution, 25°C).

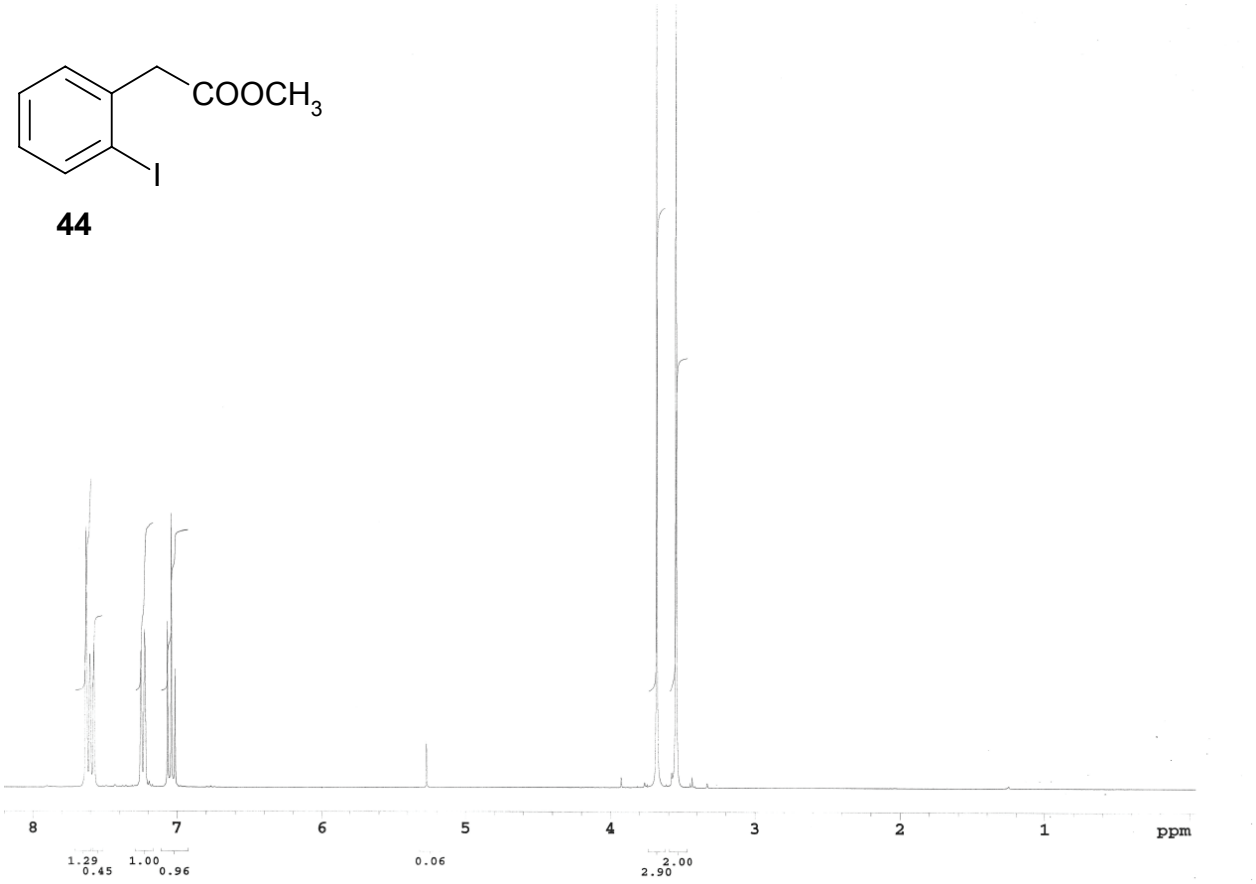

Figure S 35: ^{1}H NMR spectrum of compound **44** (300 MHz, $CDCl_3$ solution, 25°C).

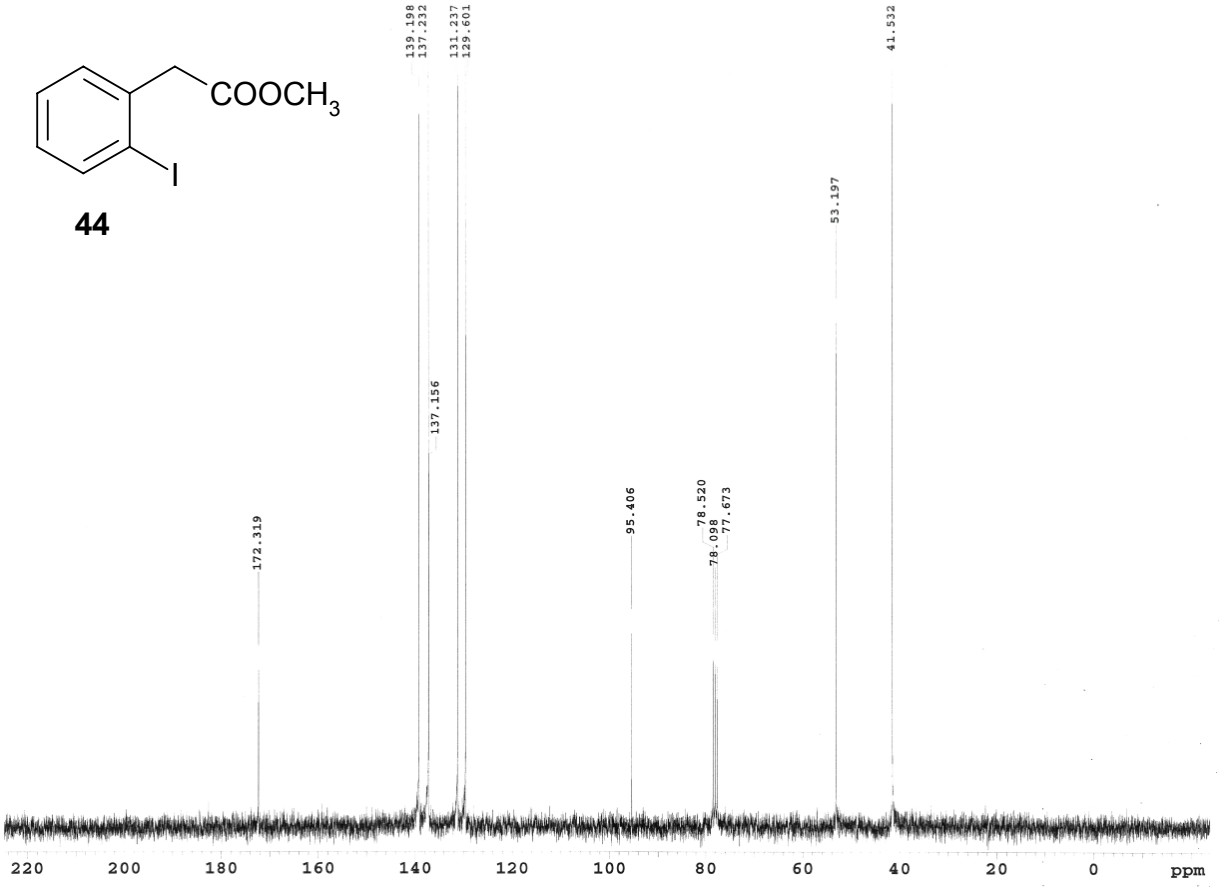

Figure S 36: ^{13}C NMR spectrum of compound **44** (75 MHz, $CDCl_3$ solution, 25°C).

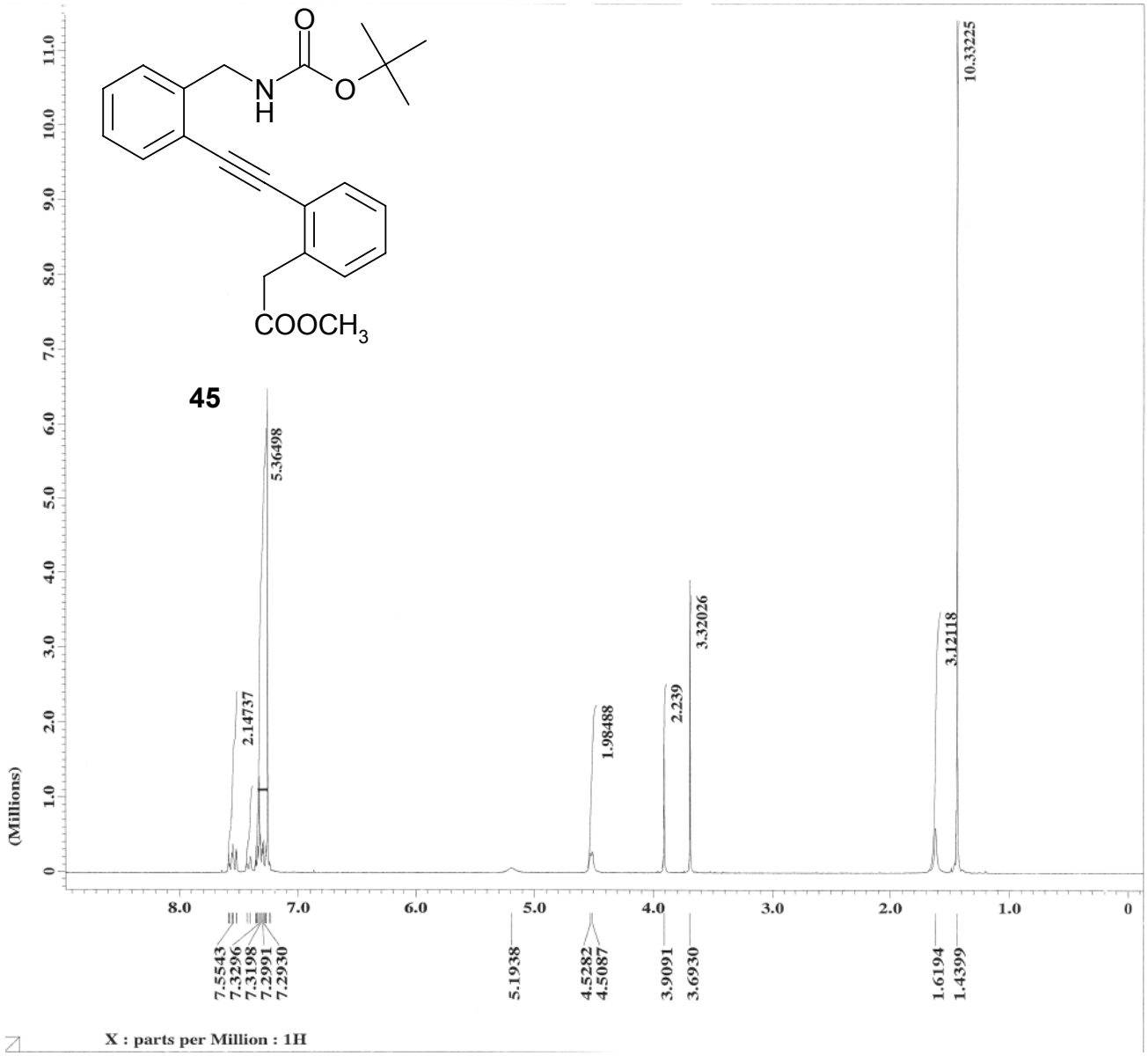

Figure S 37: ^{1}H NMR spectrum of compound **45** (270.2 MHz, $CDCl_3$ solution, 25°C).

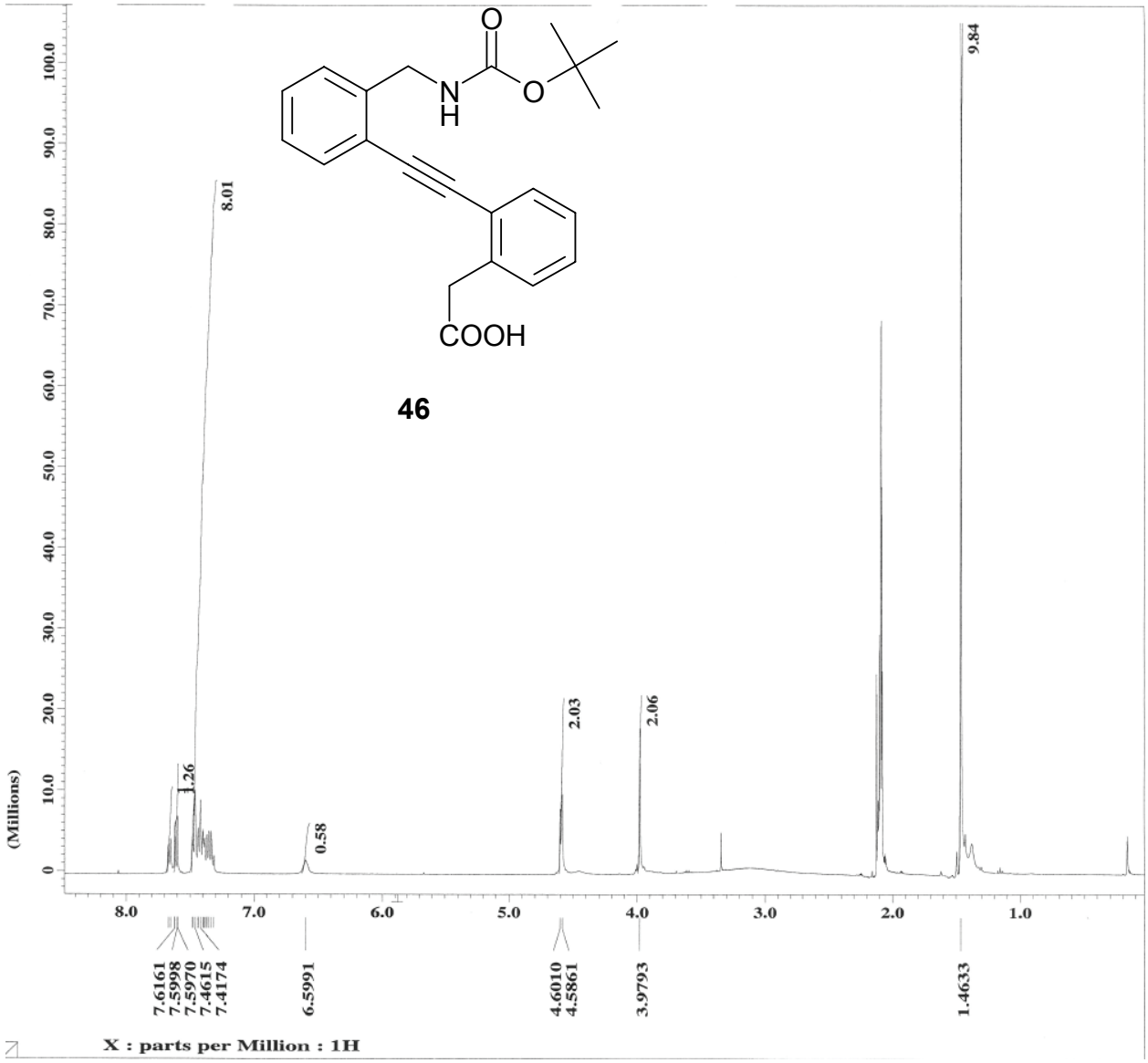

Figure S 38: ^{1}H NMR spectrum of compound **46** (399.8 MHz, acetone-d_6 solution, 25°C).

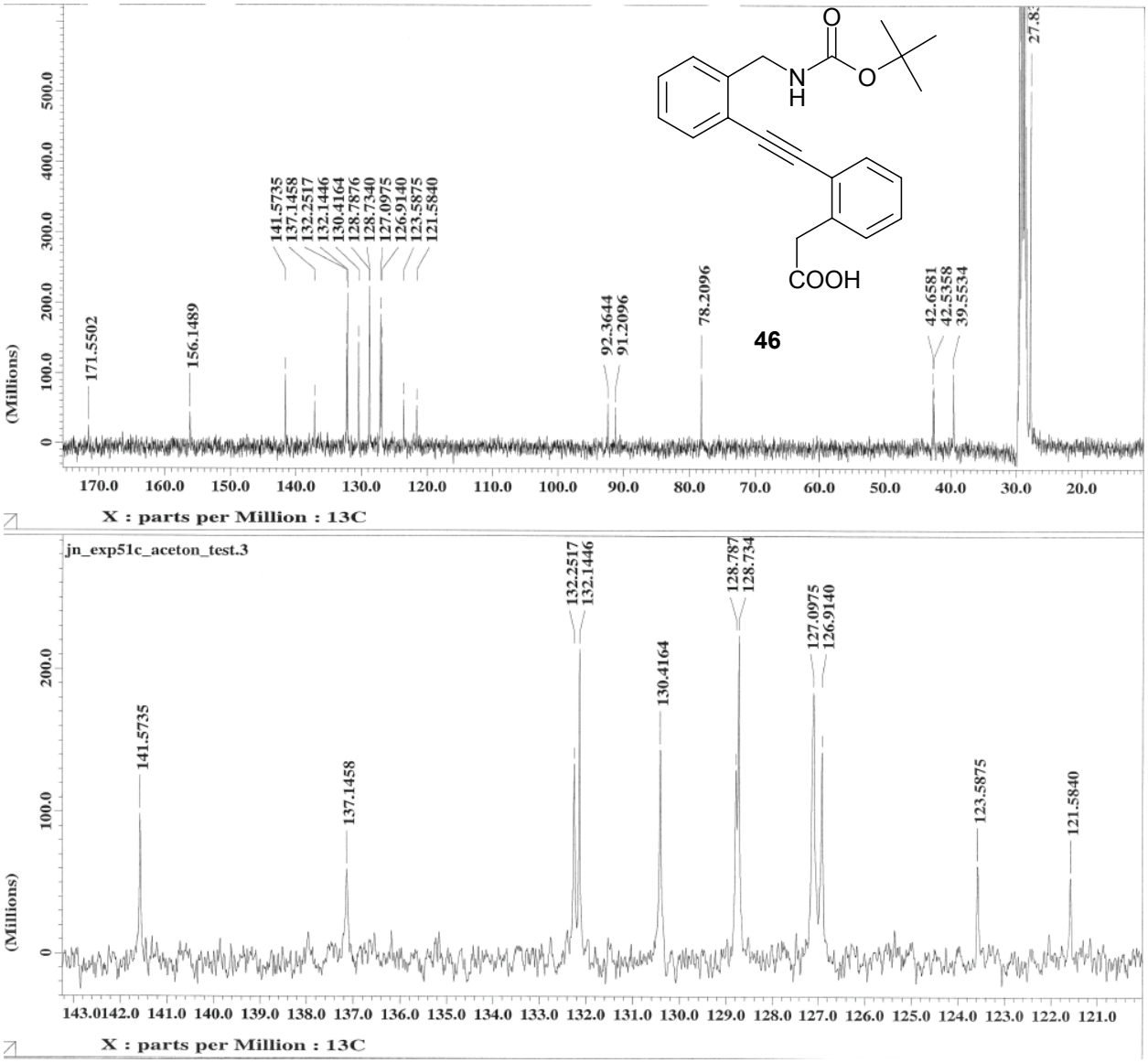

Figure S 39: ^{13}C NMR spectrum of compound **46** (100.5 MHz, acetone-d_6 solution, 25°C).