

Supplementary Material

Synthesis and physicochemical properties of merocyanine dyes based on dihydropyridine and fragments of cyanoacetic acid derivatives

Irina A. Borisova, Andrey A. Zubarev, Lydmila A. Rodinovskaya Anatoliy M. Shestopalov*

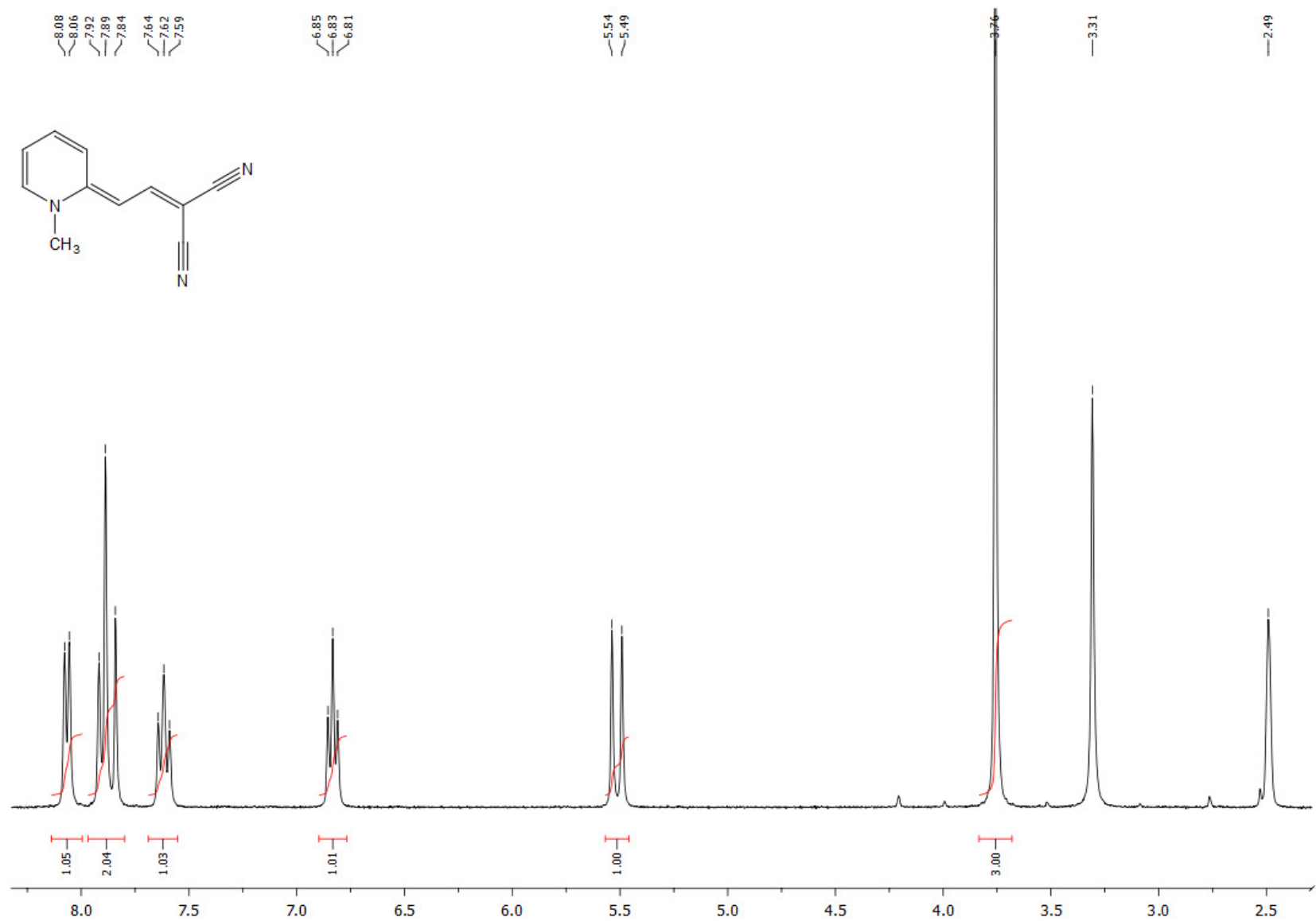
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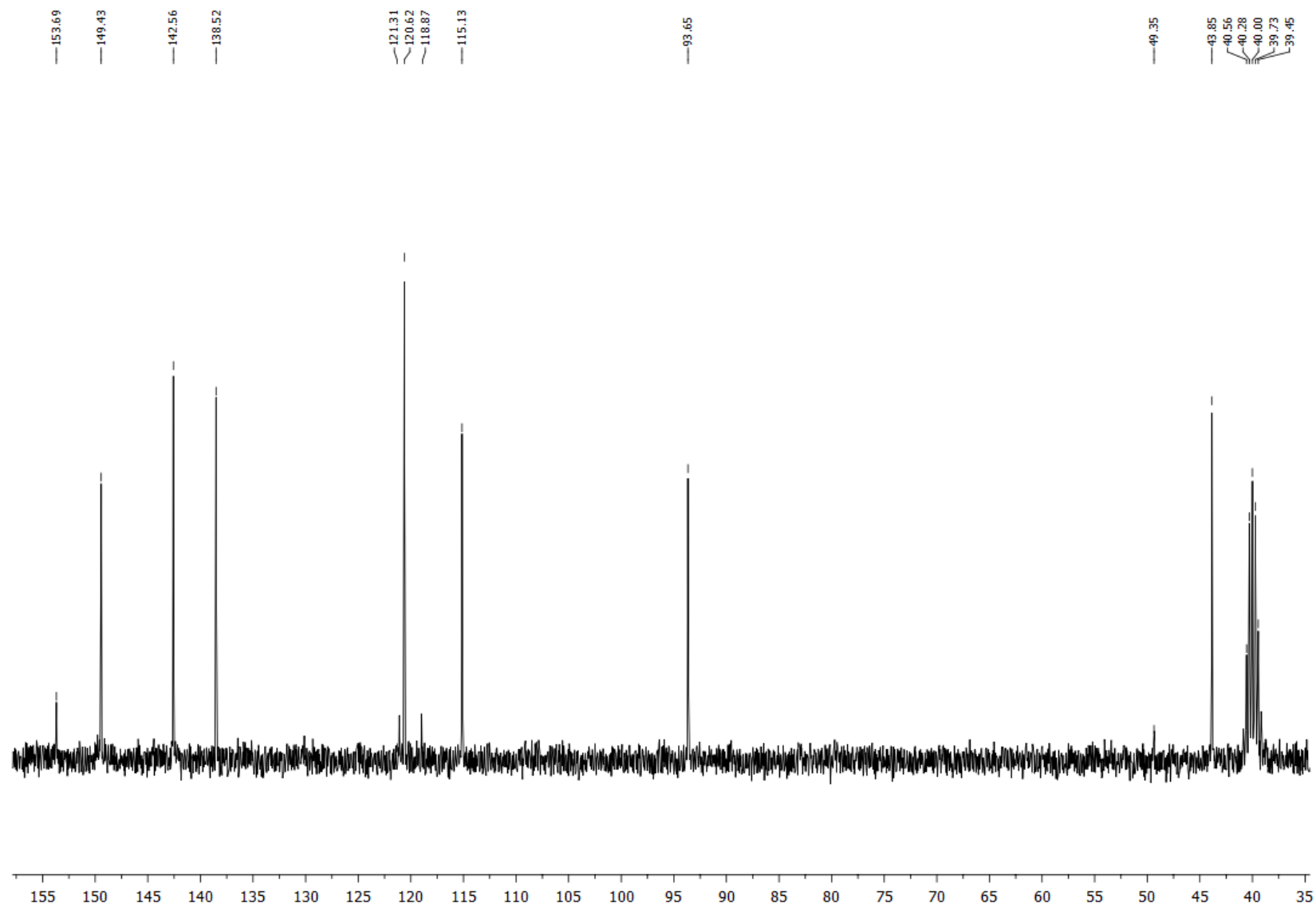
Copies of ^1H , ^{13}C NMR Spectra (300/75 MHz)

(<i>E</i>)-2-(2-(1'-Methylpyridin-2'(1' <i>H</i>))-ylidene)ethylidene)malononitrile 6a	S3
Ethyl (2 <i>E</i> ,4 <i>E</i>)-2-cyano-4-(1'-methylpyridin-2'(1' <i>H</i>))-ylidene)but-2-enoate 6b	S5
(2 <i>E</i> ,4 <i>E</i>)-2-Cyano-4-(1'-methylpyridin-2'(1' <i>H</i>))-ylidene)but-2-enethioamide 6c	S7
(<i>E</i>)-2-(2-(1'-Butylpyridin-2'(1' <i>H</i>))-ylidene)ethylidene)malononitrile 6d	S9
Ethyl (2 <i>E</i> ,4 <i>E</i>)-2-cyano-4-(1'-butylpyridin-2'(1' <i>H</i>))-ylidene)but-2-enoate 6e	S11
(2 <i>E</i> ,4 <i>E</i>)-4-(1'-Butylpyridin-2'(1' <i>H</i>))-ylidene)-2-cyanobut-2-enethioamide 6f	S13
(<i>E</i>)-2-(2-(1'-Octylpyridin-2'(1' <i>H</i>))-ylidene)ethylidene)malononitrile 6g	S15
Ethyl (2 <i>E</i> ,4 <i>E</i>)-2-cyano-4-(1'-octylpyridin-2'(1' <i>H</i>))-ylidene)but-2-enoate 6h	S17
(2 <i>E</i> ,4 <i>E</i>)-4-(1'-Octylpyridin-2'(1' <i>H</i>))-ylidene)-2-cyanobut-2-enethioamide 6i	S19
<i>tert</i> -Butyl (<i>E</i>)-2-(2-(3,3-dicyanoallylidene)pyridin-1(2 <i>H</i>))-yl)acetate 6j	S21
Ethyl (2 <i>E</i> ,4 <i>E</i>)-4-(1-(2-(<i>tert</i> -butoxy)-2-oxoethyl)pyridin-1(2 <i>H</i>))-ylidene)-2-cyanobut-2-enoate 6k	S23

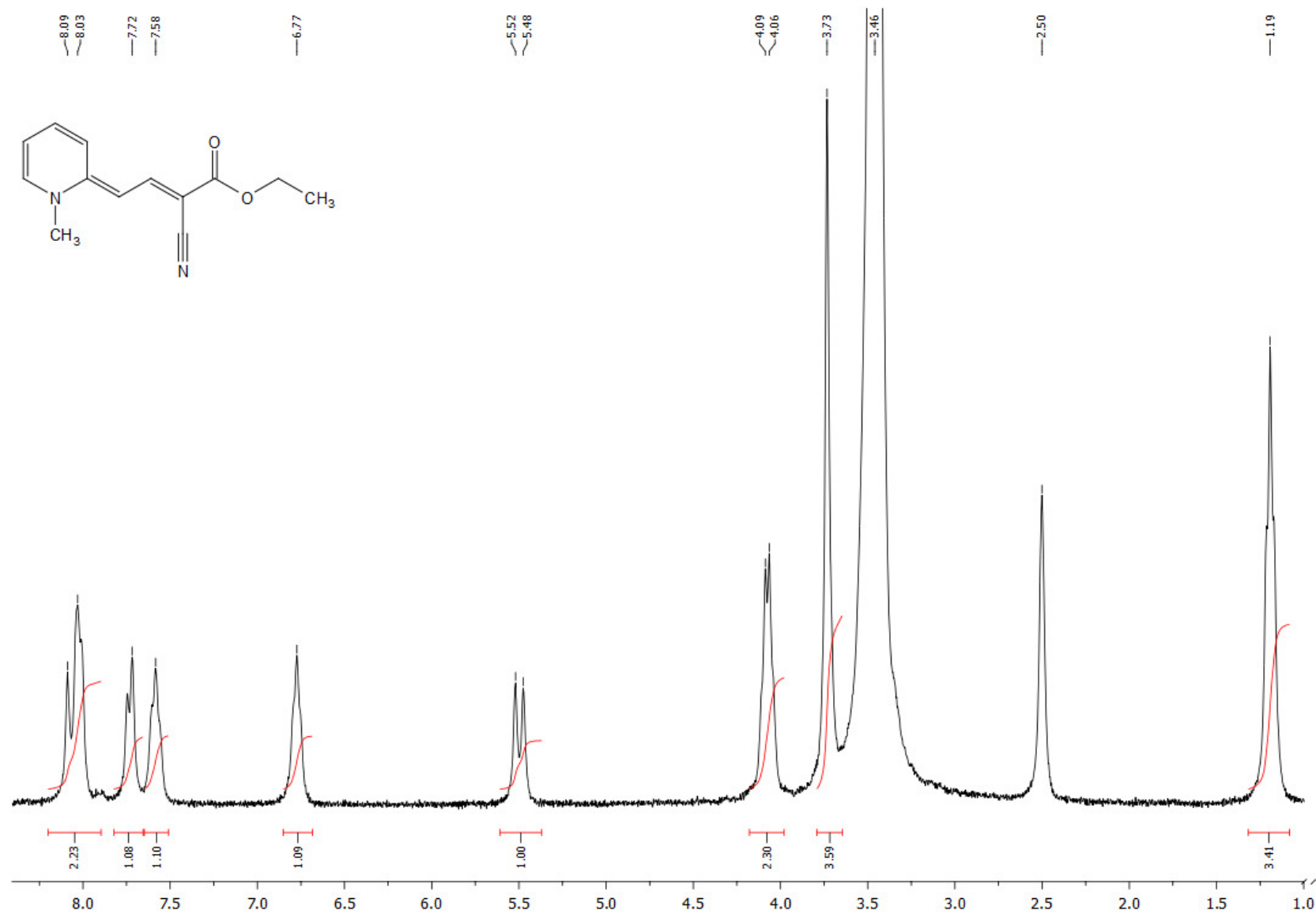
<i>tert</i> -Butyl 2-((<i>E</i>)-2-((<i>E</i>)-4-amino-3-cyano-4-thioxobut-2-en-1-ylidene)pyridin-1(2 <i>H</i>)-yl)acetate 6l	S25
2-(2-(1'-Methylpyridin-4'(1' <i>H</i>)-ylidene)ethylidene)malononitrile 7a	S27
Ethyl (<i>Z</i>)-2-cyano-4-(1'-methylpyridin-4'(1' <i>H</i>)-ylidene)but-2-enoate 7b	S29
(<i>Z</i>)-2-Cyano-4-(1'-methylpyridin-4'(1' <i>H</i>)-ylidene)but-2-enethioamide 7c	S31
2-(2-(1'-Butylpyridin-4'(1' <i>H</i>)-ylidene)ethylidene)malononitrile 7d	S33
Ethyl (<i>Z</i>)-2-cyano-4-(1-butylpyridin-4(1 <i>H</i>)-ylidene)but-2-enoate 7e	S35
(<i>Z</i>)-2-Cyano-4-(1'-butylpyridin-4'(1' <i>H</i>)-ylidene)but-2-enethioamide 7f	S37
2-(2-(1'-Octylpyridin-4'(1' <i>H</i>)-ylidene)ethylidene)malononitrile 7g	S39
Ethyl (<i>Z</i>)-2-cyano-4-(1'-octylpyridin-4'(1' <i>H</i>)-ylidene)but-2-enoate 7h	S41
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¹ H, ¹³ C, ¹³ C DEPT, COSY, 2D HSQC Spectra of 2-(3,3-dicyanoallyl)-1-methylpyridin-1-ium 2,2,2-trifluoroacetate 6a.1	S45



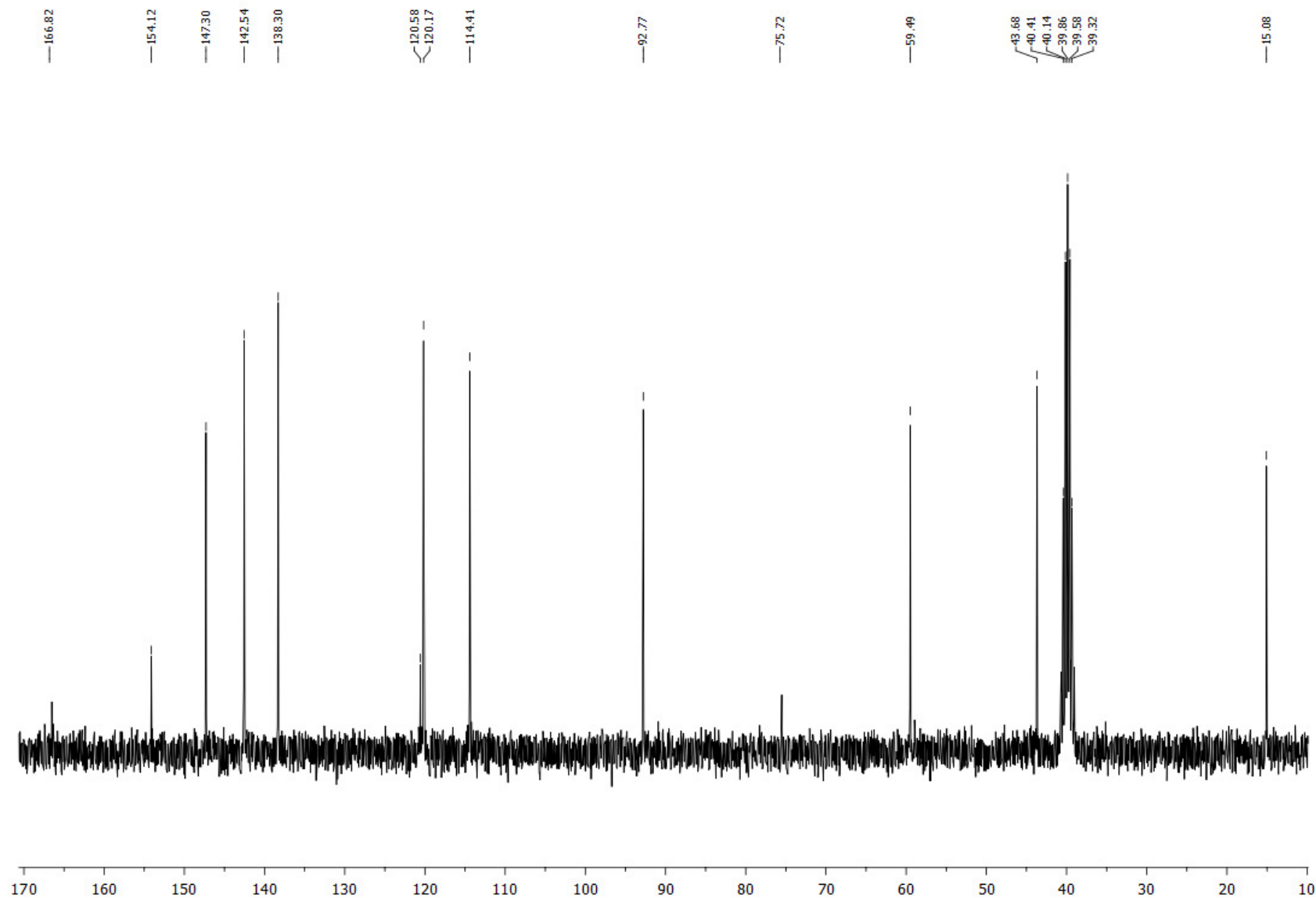
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of (*E*)-2-(2-(1'-Methylpyridin-2' (1'*H*)-ylidene)ethylidene)malononitrile **6a**



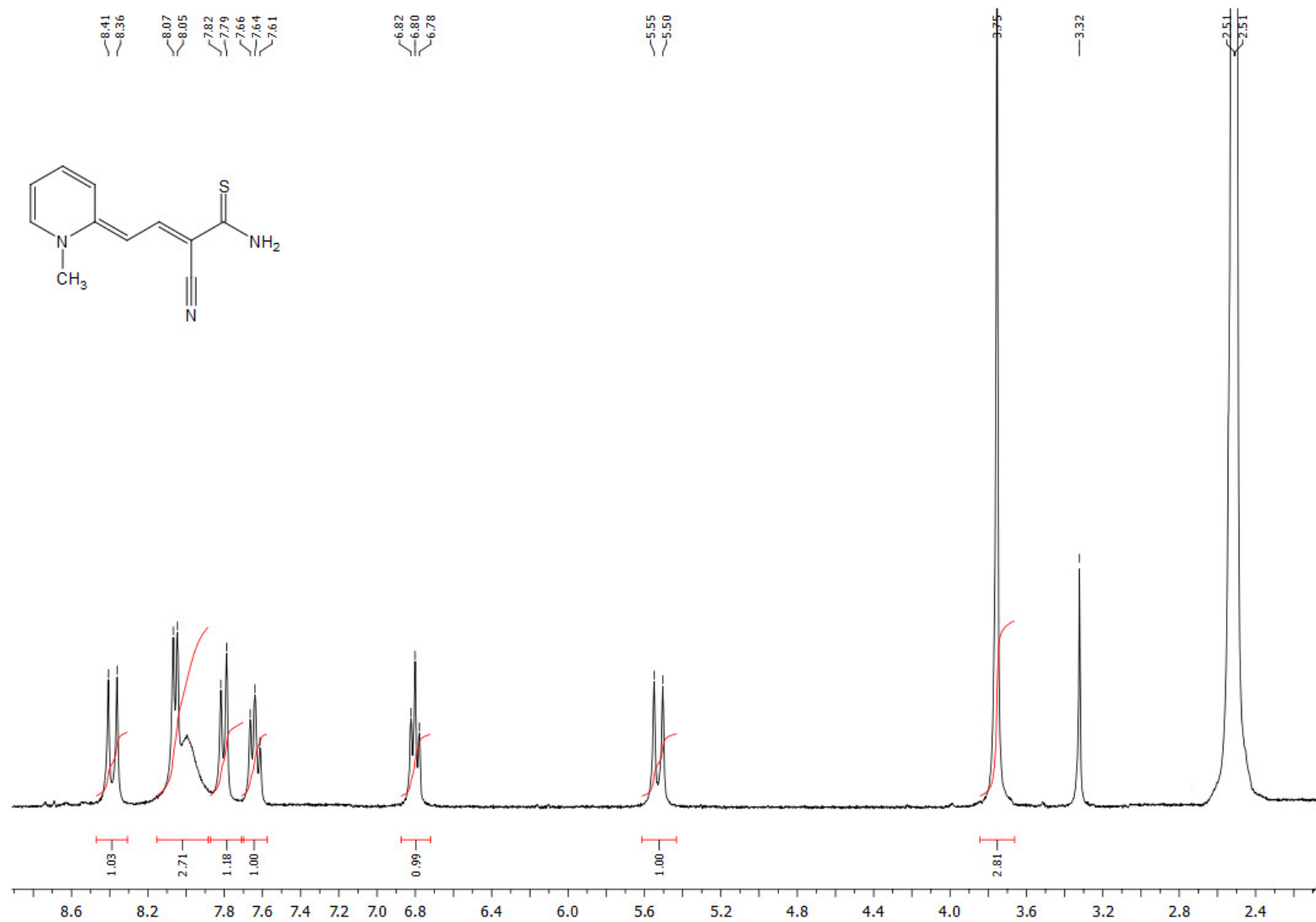
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of (E)-2-(2-(1'-Methylpyridin-2' (1'*H*)-ylidene)ethylidene)malononitrile **6a**



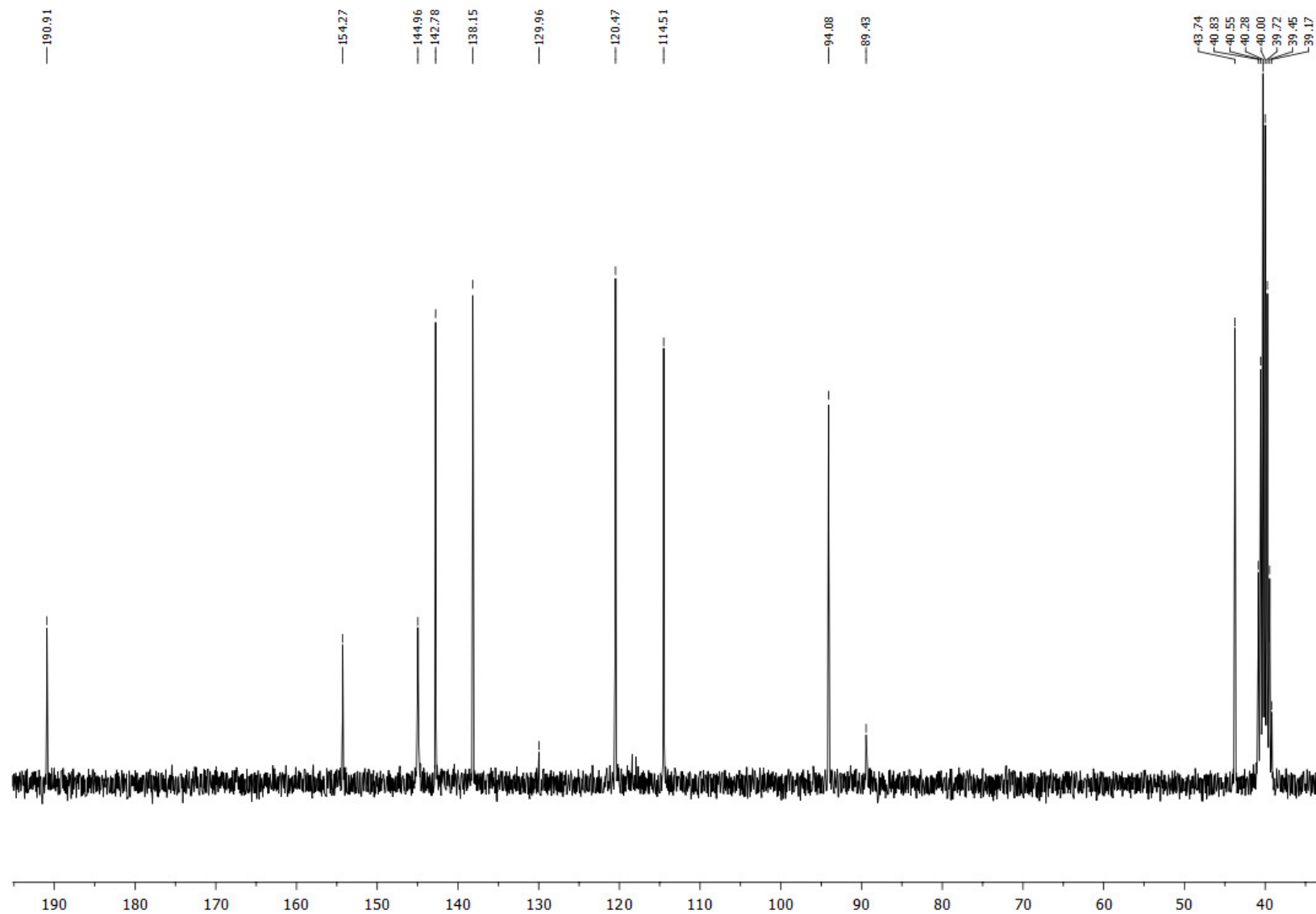
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of ethyl (2*E*,4*E*)-2-cyano-4-(1'-methylpyridin-2'(1'*H*)-ylidene)but-2-enoate **6b**



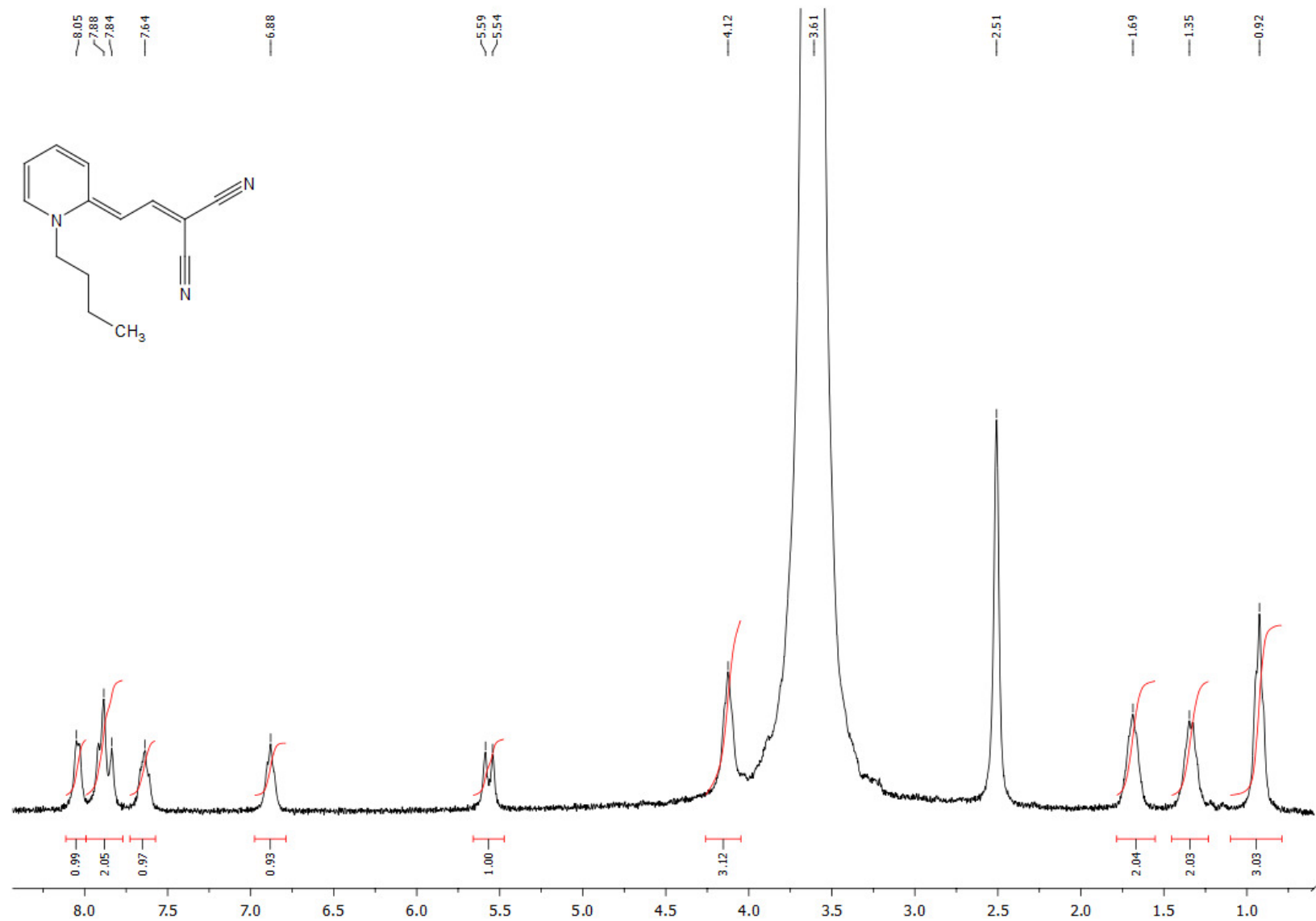
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of ethyl (2*E*,4*E*)-2-cyano-4-(1'-methylpyridin-2'(1'*H*)-ylidene)but-2-enoate **6b**



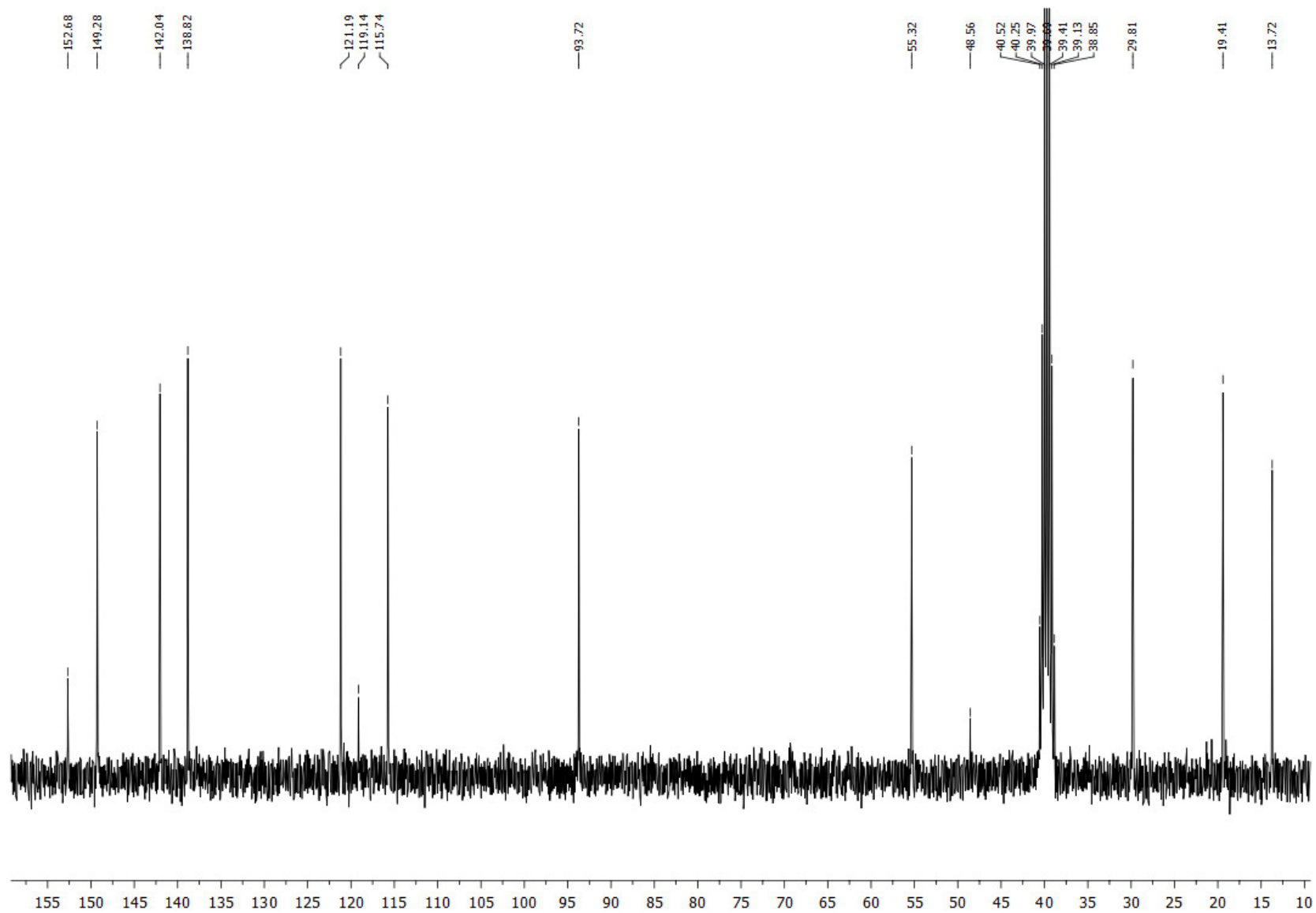
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of (2*E*,4*E*)-2-cyano-4-(1'-methylpyridin-2'(1'*H*)-ylidene)but-2-enethioamide **6c**



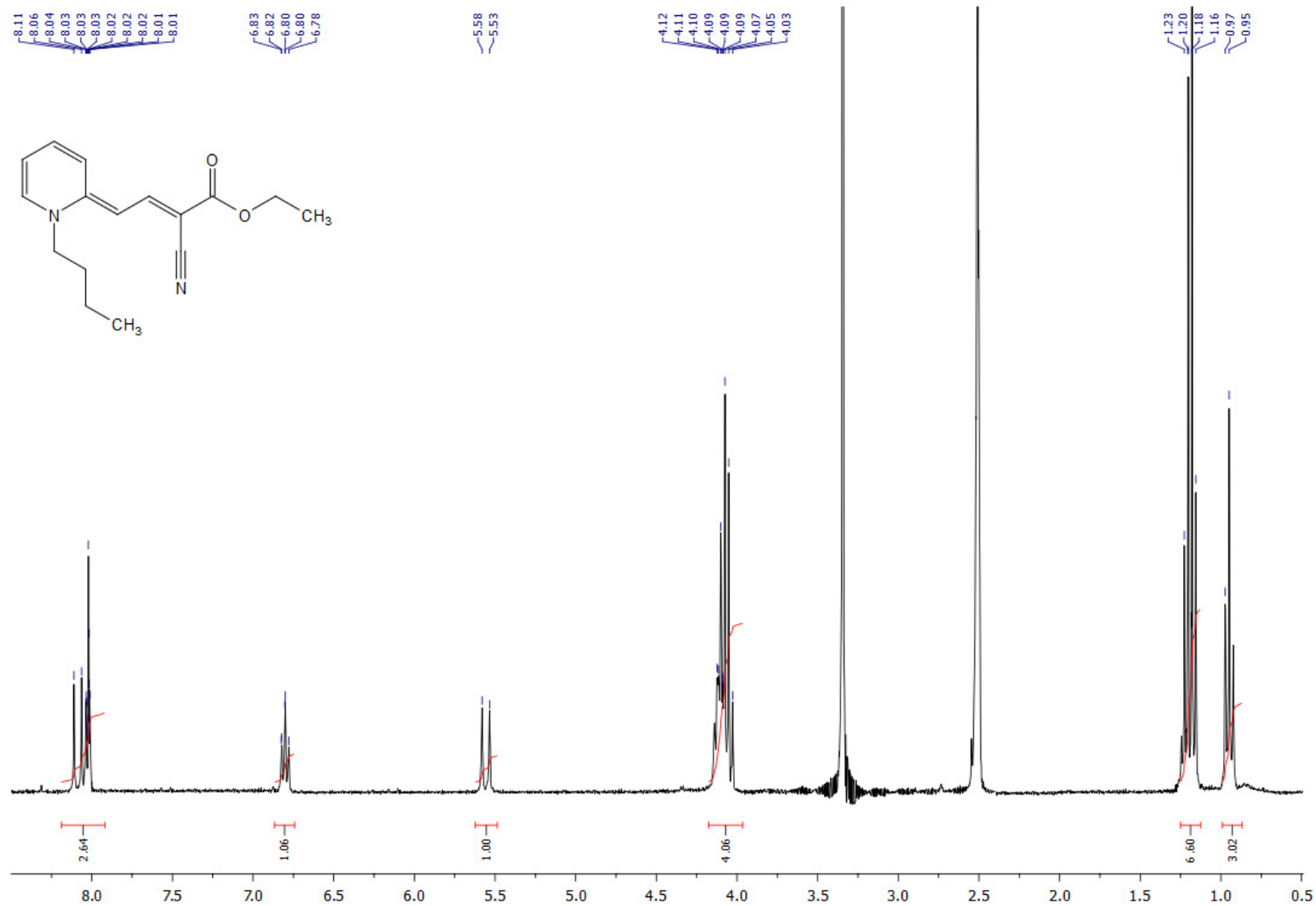
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of $(2E,4E)$ -2-cyano-4-(1'-methylpyridin-2'(1'*H*)-ylidene)but-2-enethioamide **6c**



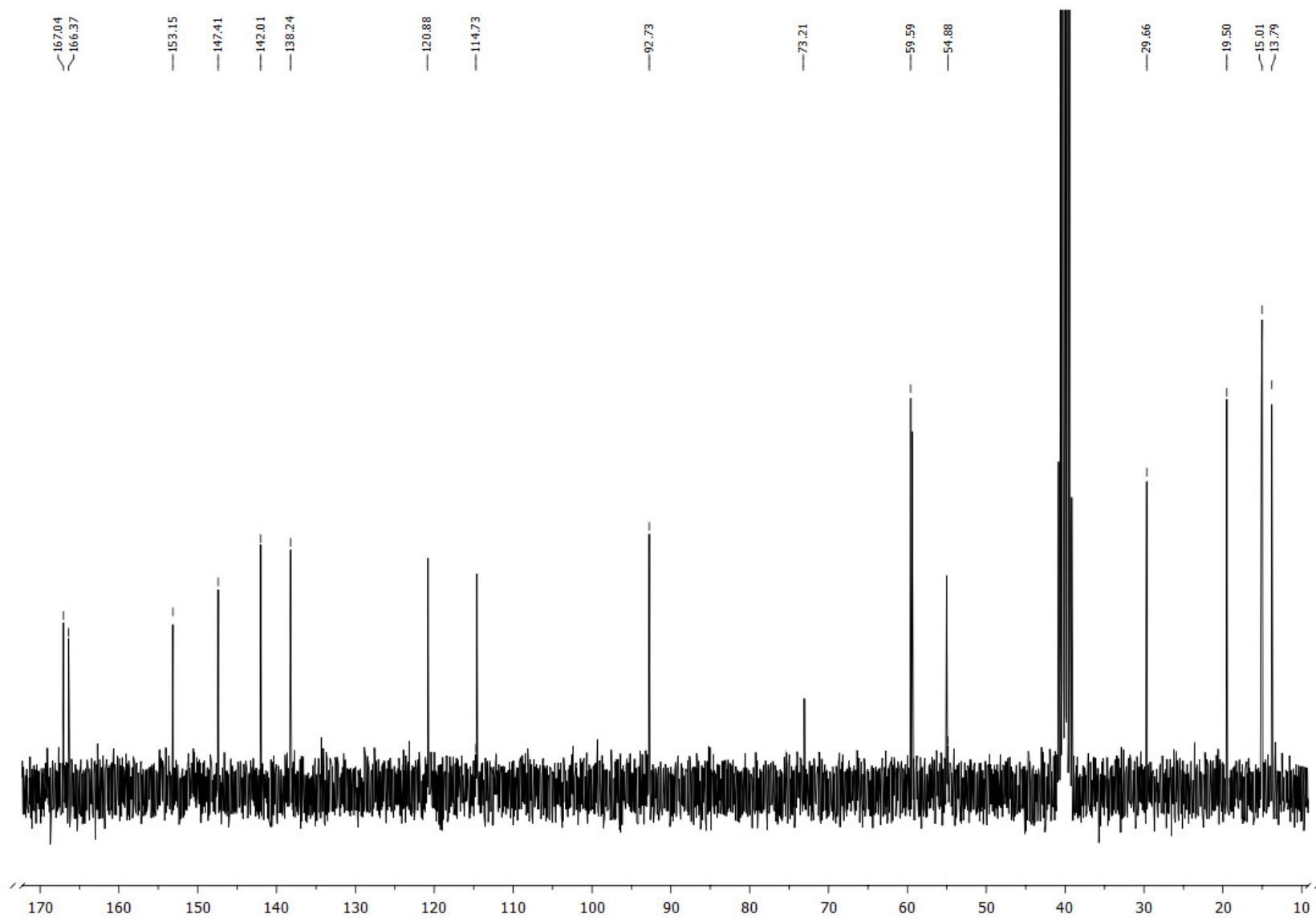
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of (*E*)-2-(2-(1'-butylpyridin-2'(1'*H*)-ylidene)ethylidene)malononitrile **6d**



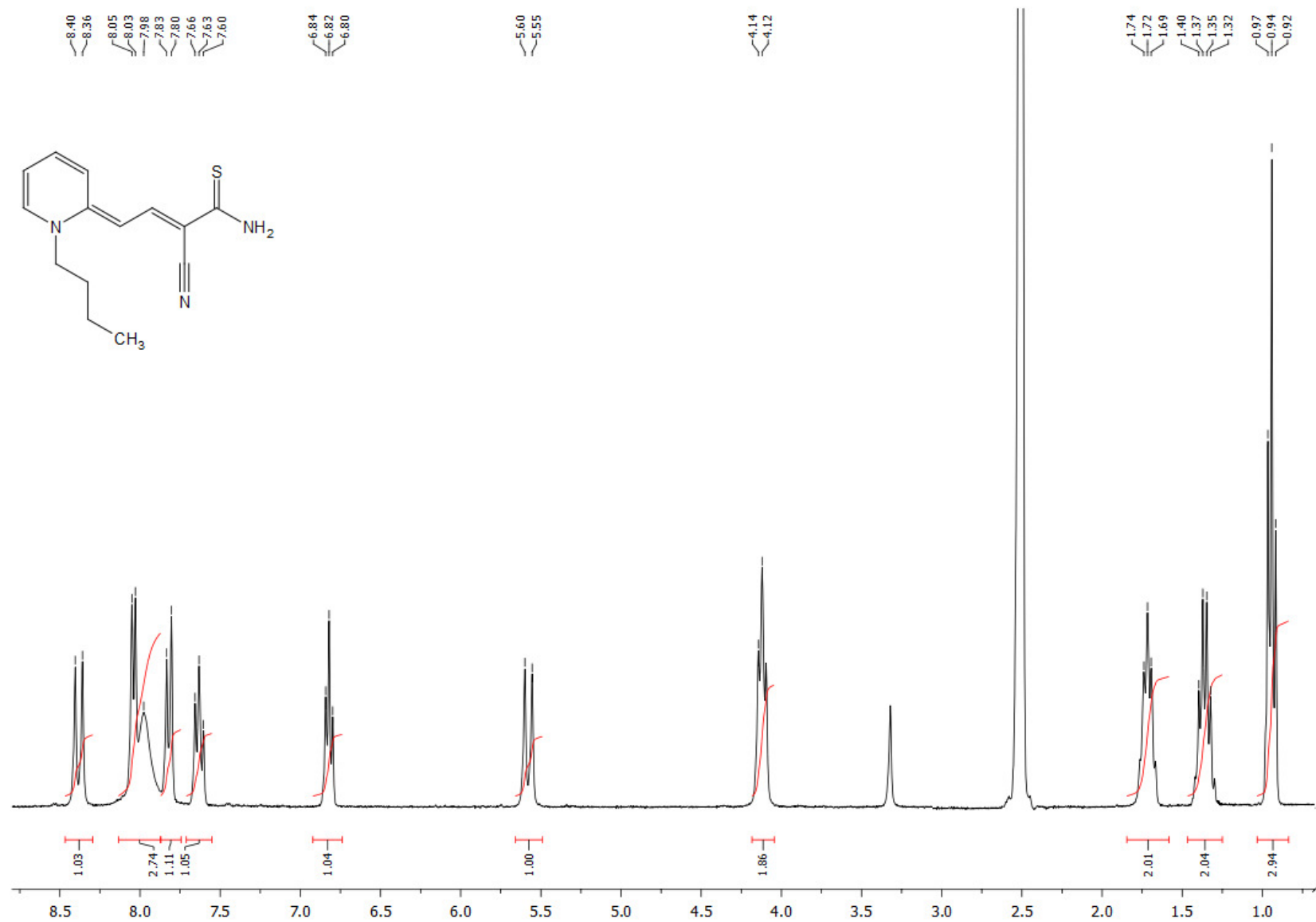
¹³C NMR (75.5 MHz, DMSO-*d*₆) spectrum of (*E*)-2-(2-(1'-butylpyridin-2'(1*H*)-ylidene)ethylidene)malononitrile **6d**



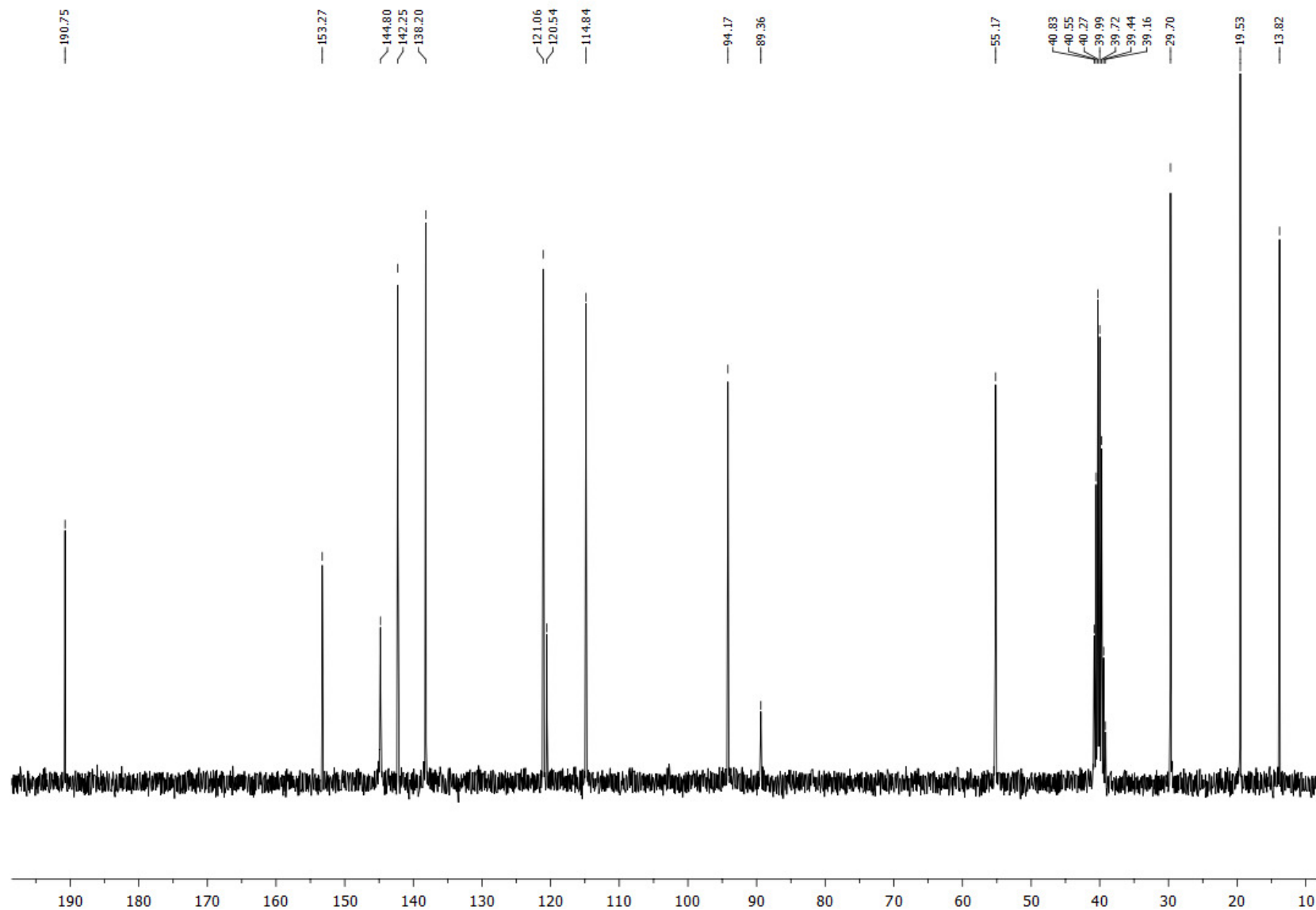
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of ethyl (2E,4E)-2-cyano-4-(1'-butylpyridin-2'(1'H)-ylidene)but-2-enoate **6e**



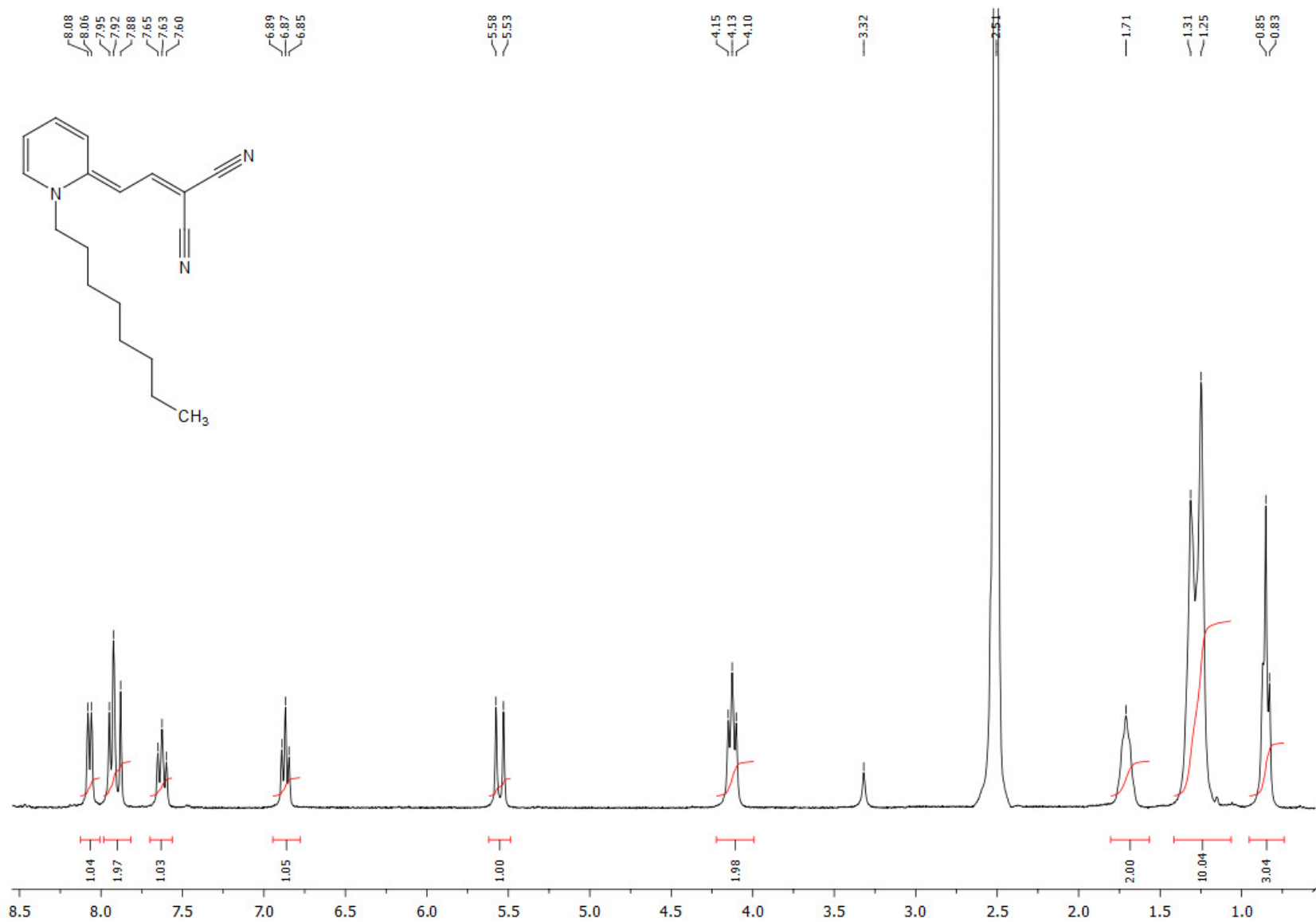
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of ethyl (2*E*,4*E*)-2-cyano-4-(1'-butylpyridin-2'(1'*H*)-ylidene)but-2-enoate **6e**



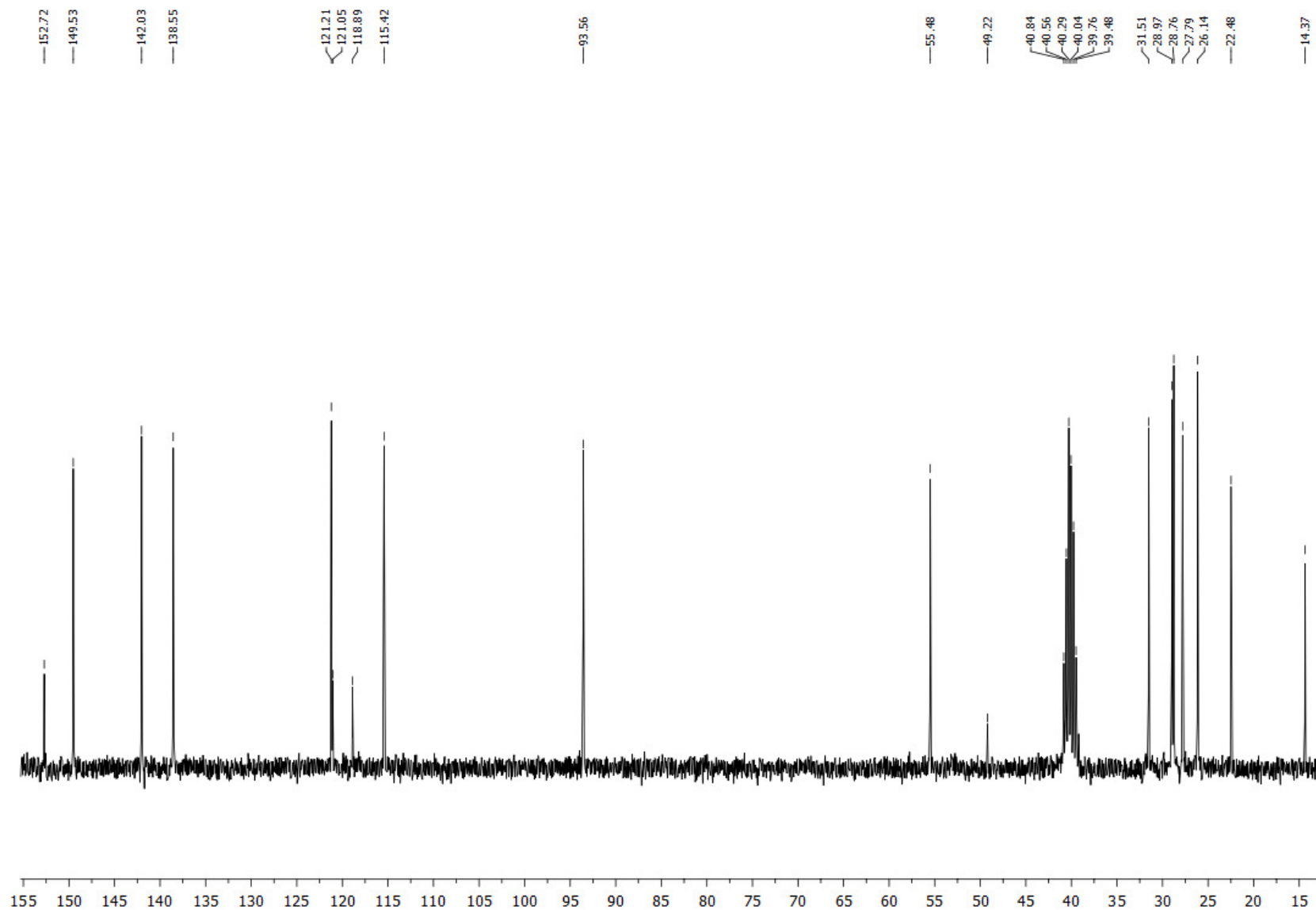
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of (2E,4E)-4-(1'-butylpyridin-2'(1'H)-ylidene)-2-cyanobut-2-enethioamide **6f**



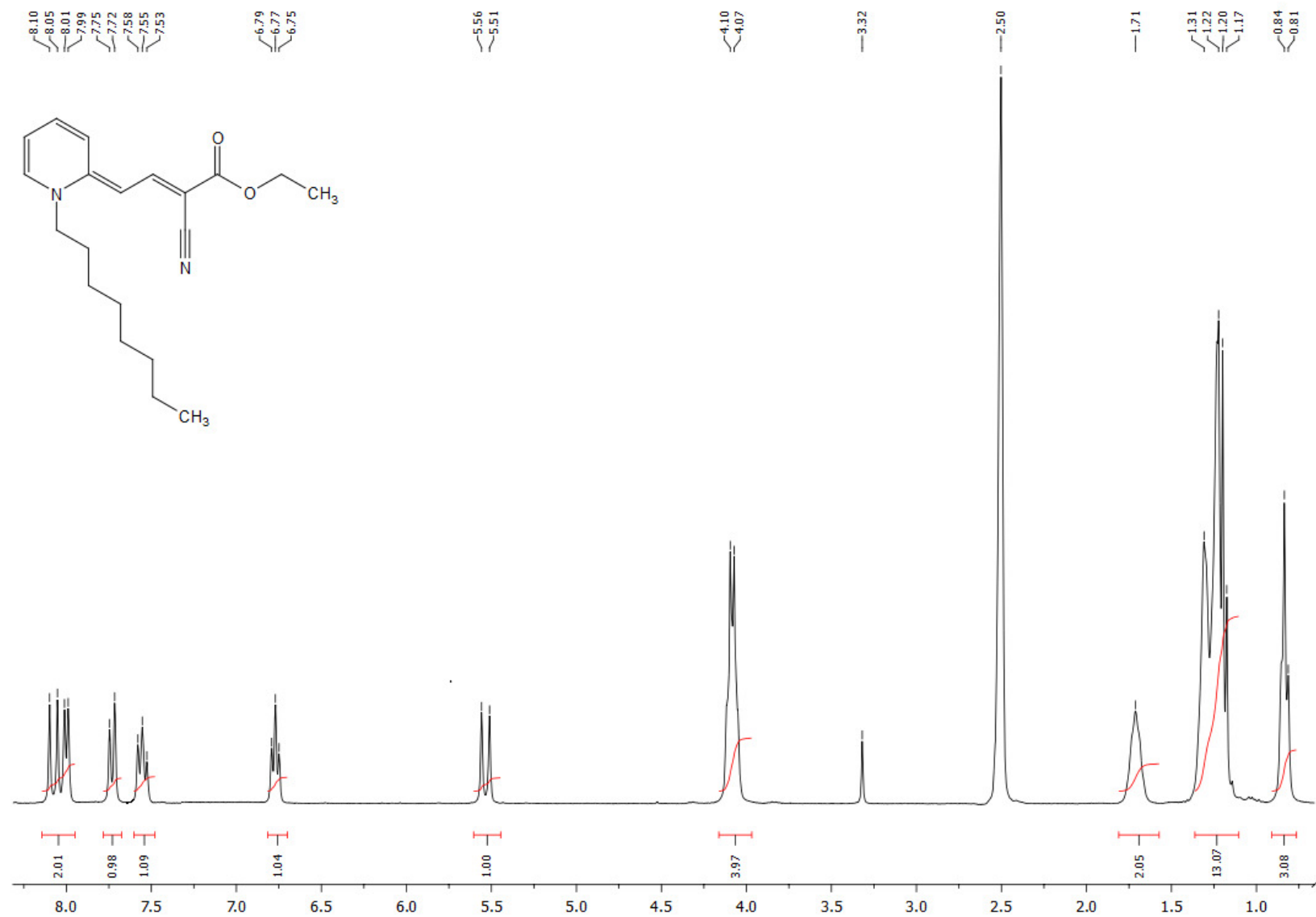
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of (2E,4E)-4-(1'-butylpyridin-2'(1'H)-ylidene)-2-cyanobut-2-enethioamide **6f**



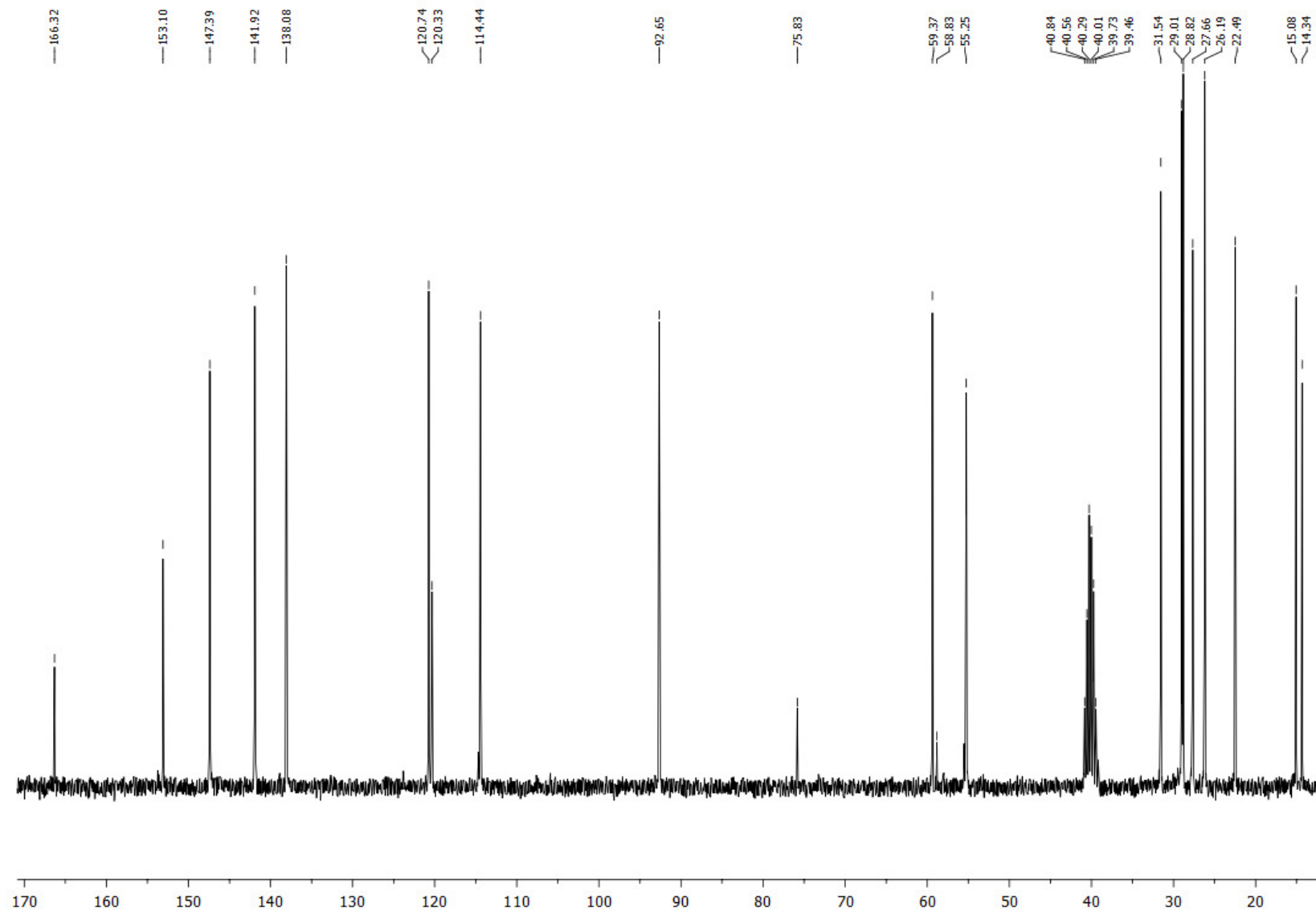
^1H NMR (300.1MHz, $\text{DMSO-}d_6$) spectrum of (E)-2-(2-(1'-octylpyridin-2'(1'H)-ylidene)ethylidene)malononitrile **6g**



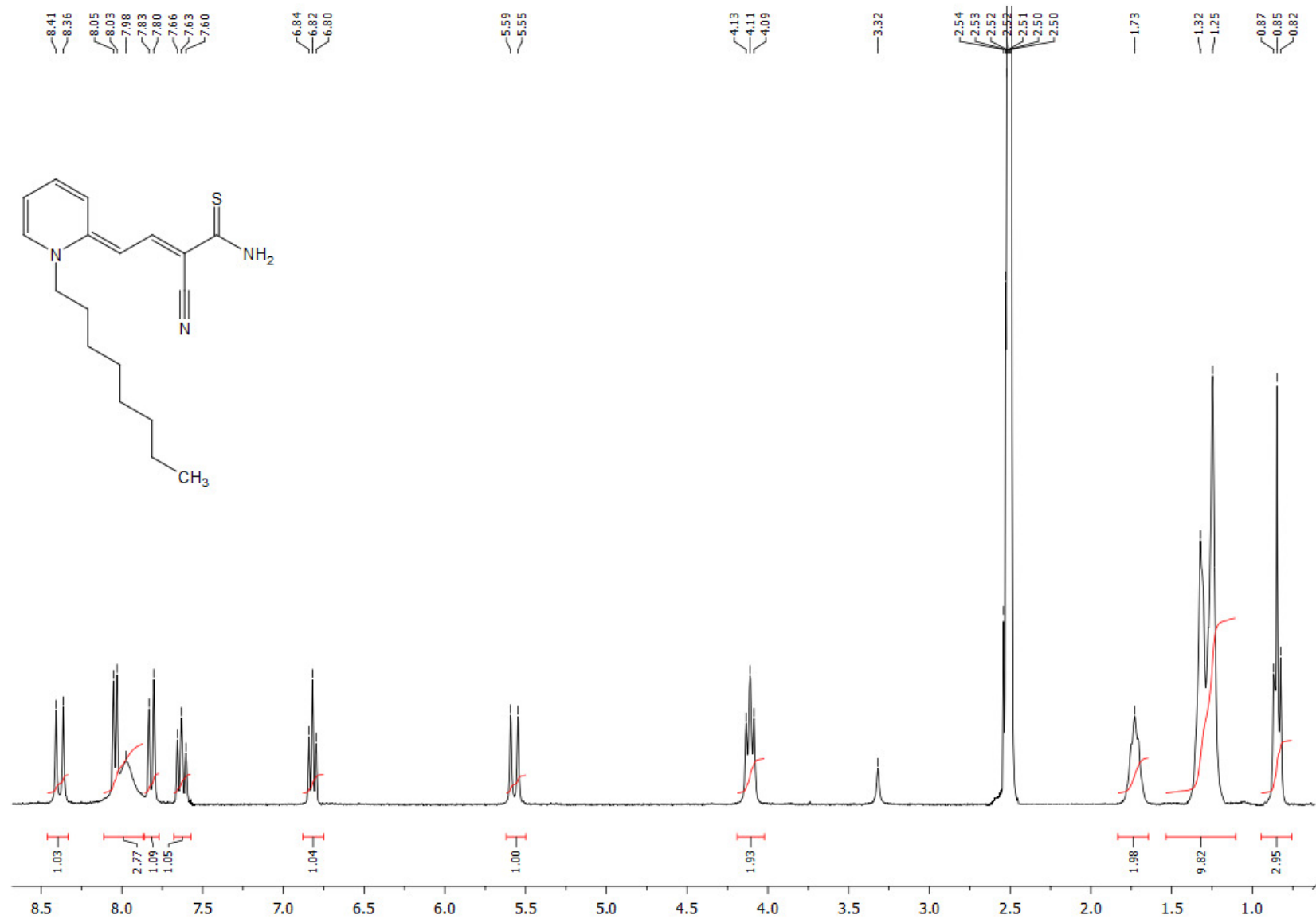
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of (E)-2-(2-(1'-octylpyridin-2'(1'H)-ylidene)ethylidene)malononitrile **6g**



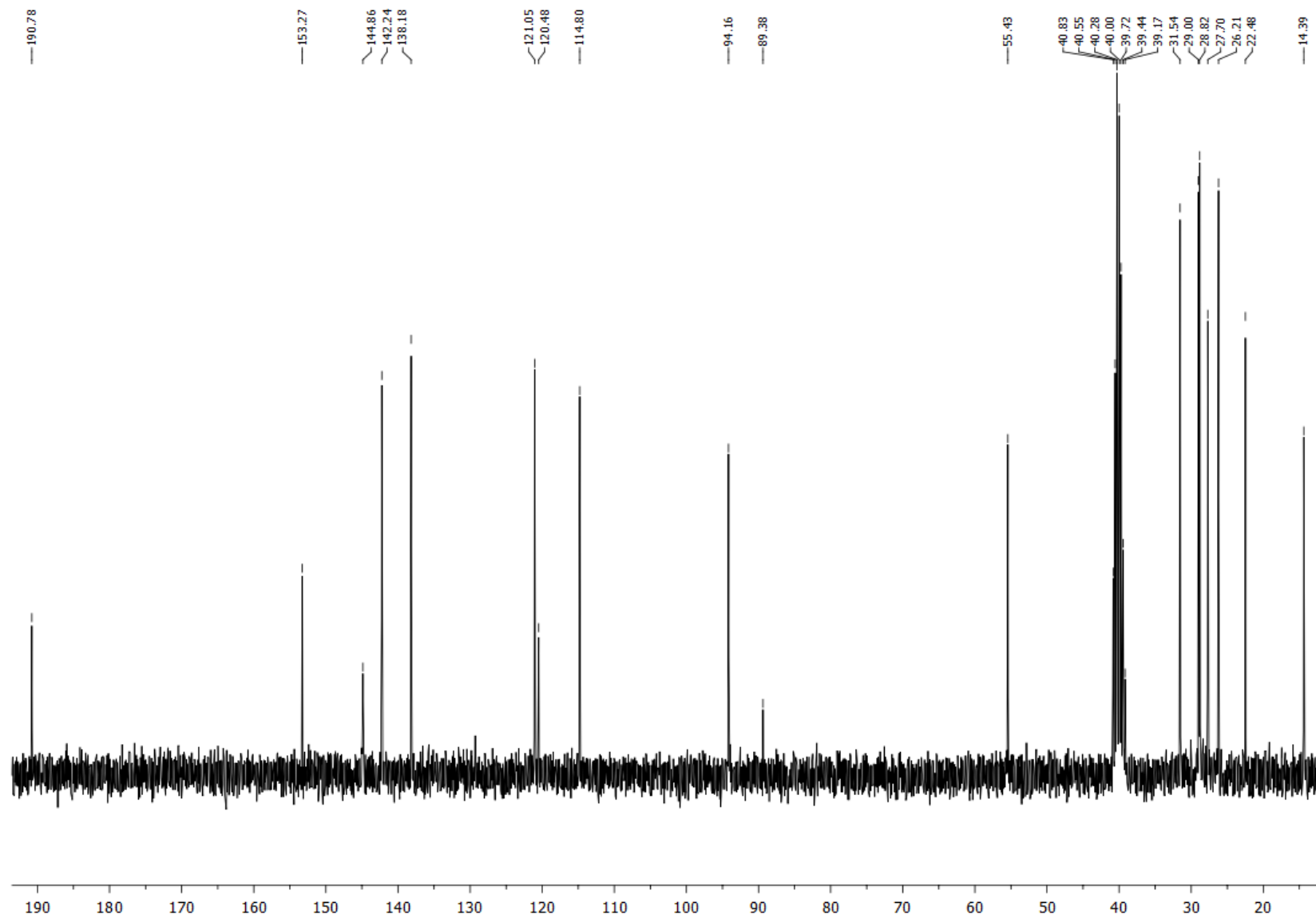
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of ethyl (2E,4E)-2-cyano-4-(1'-octylpyridin-2'(1'H)-ylidene)but-2-enoate **6h**



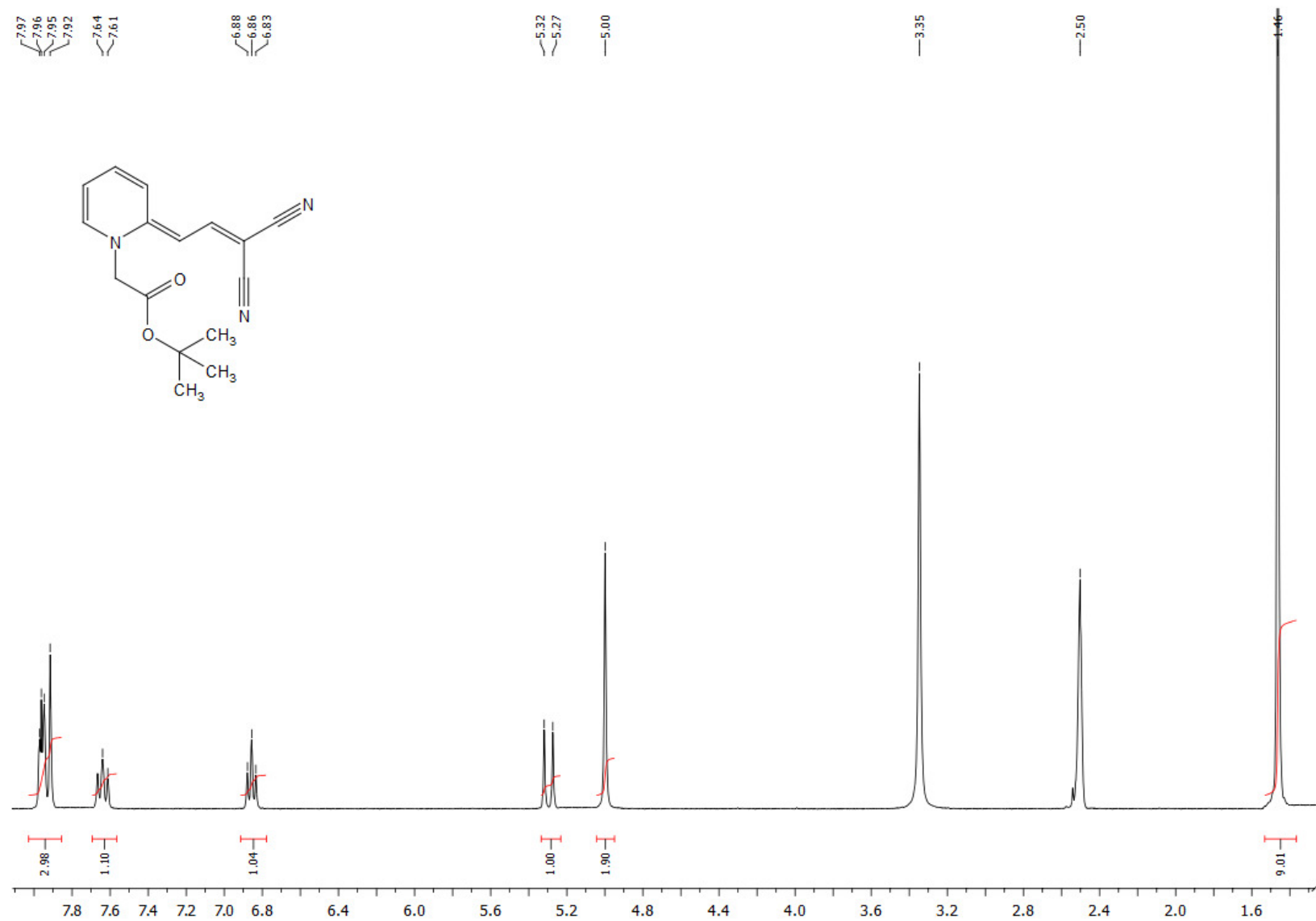
¹³C NMR (75.5 MHz, DMSO-*d*₆) spectrum of ethyl (2E,4E)-2-cyano-4-(1'-octylpyridin-2'(1'H)-ylidene)but-2-enoate **6h**



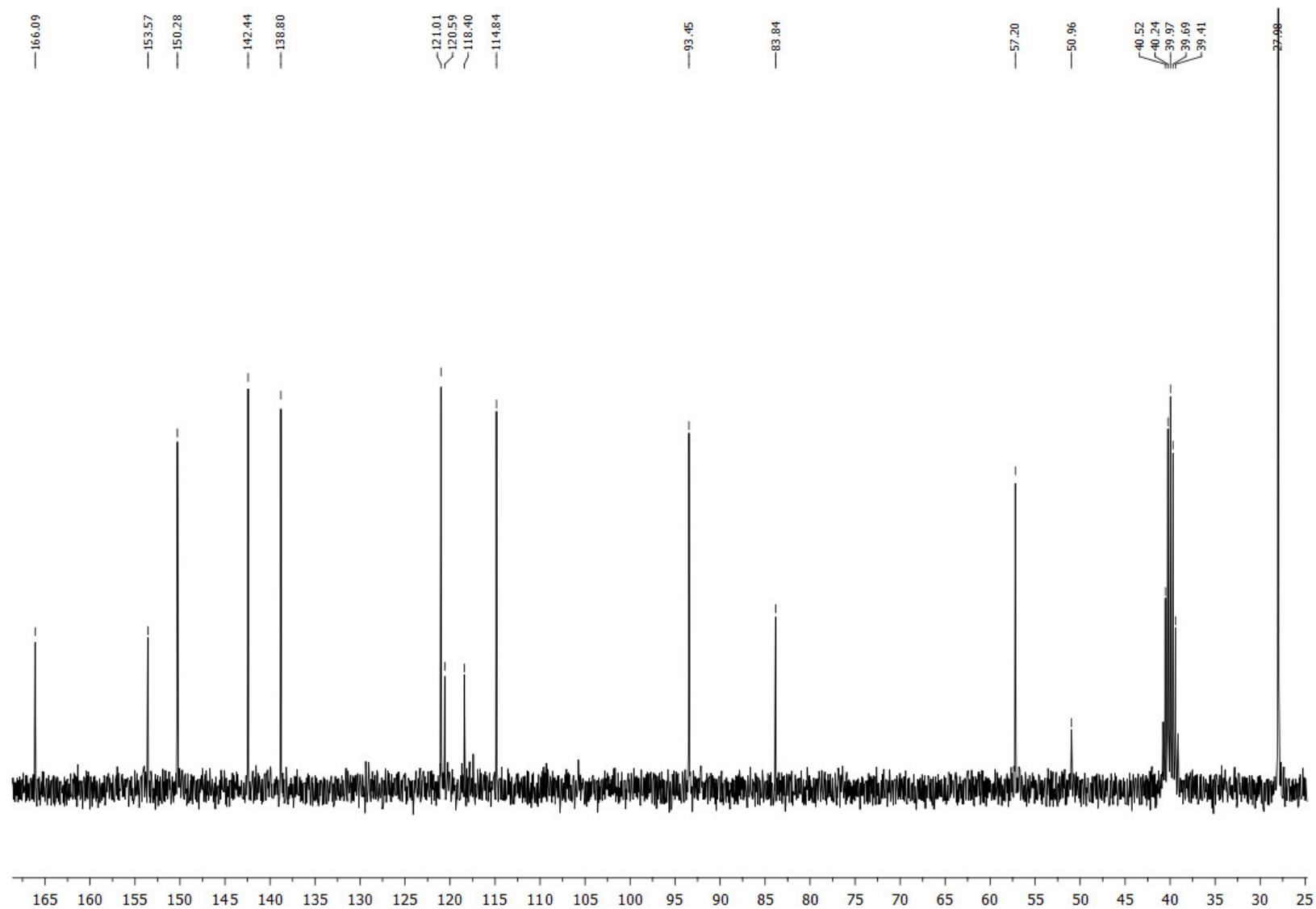
^1H NMR (300.1 MHz, $\text{DMSO-}d_6$) spectrum of (2E,4E)-4-(1'-octylpyridin-2'(1'H)-ylidene)-2-cyanobut-2-enethioamide **6i**



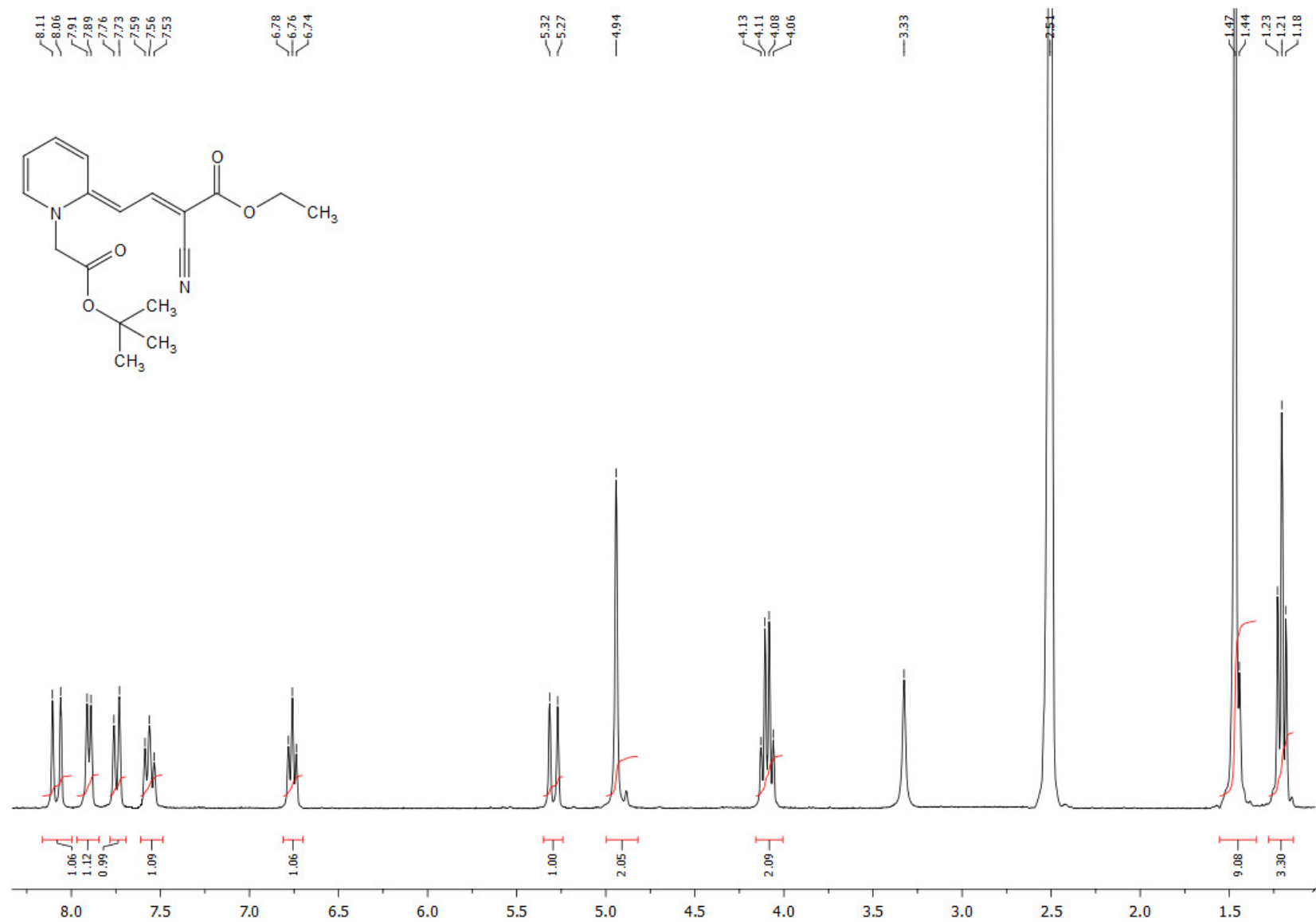
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of (2E,4E)-4-(1'-octylpyridin-2'(1'H)-ylidene)-2-cyanobut-2-enethioamide **6i**



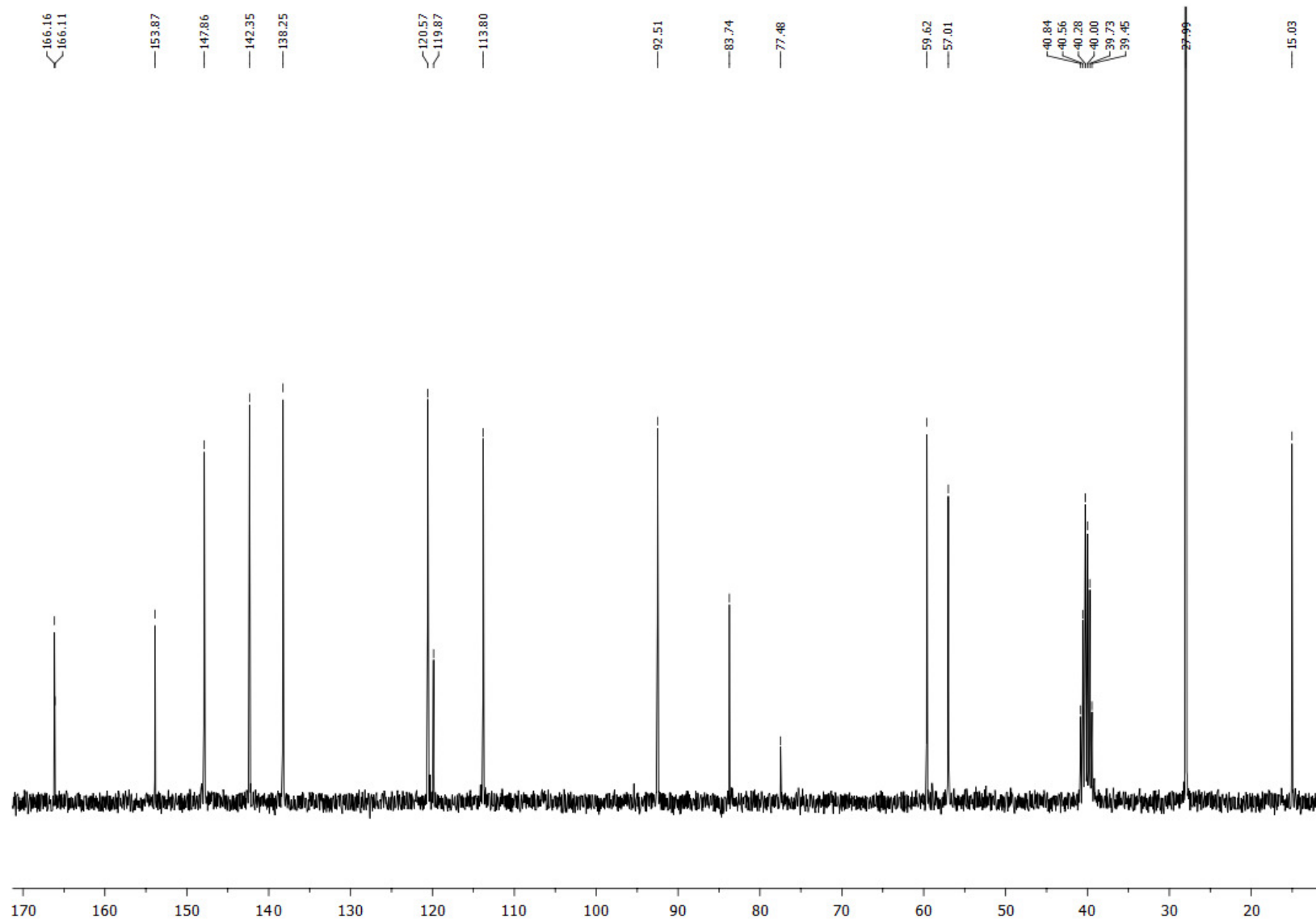
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of *tert*-butyl (E)-2-(2-(3,3-dicyanoallylidene)pyridin-1(2H)-yl)acetate **6j**



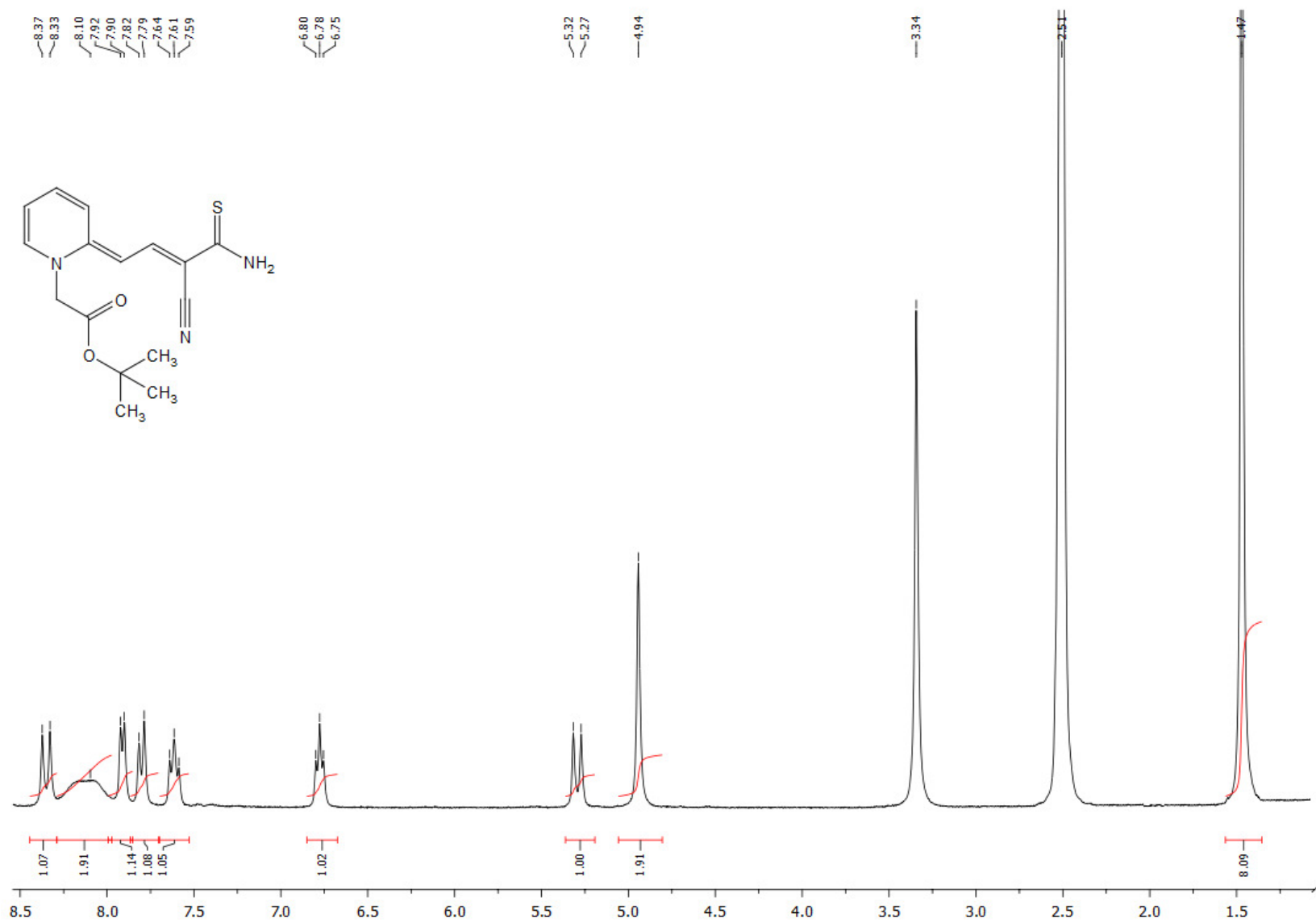
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of *tert*-butyl (E)-2-(2-(3,3-dicyanoallylidene)pyridin-1(2H)-yl)acetate **6j**



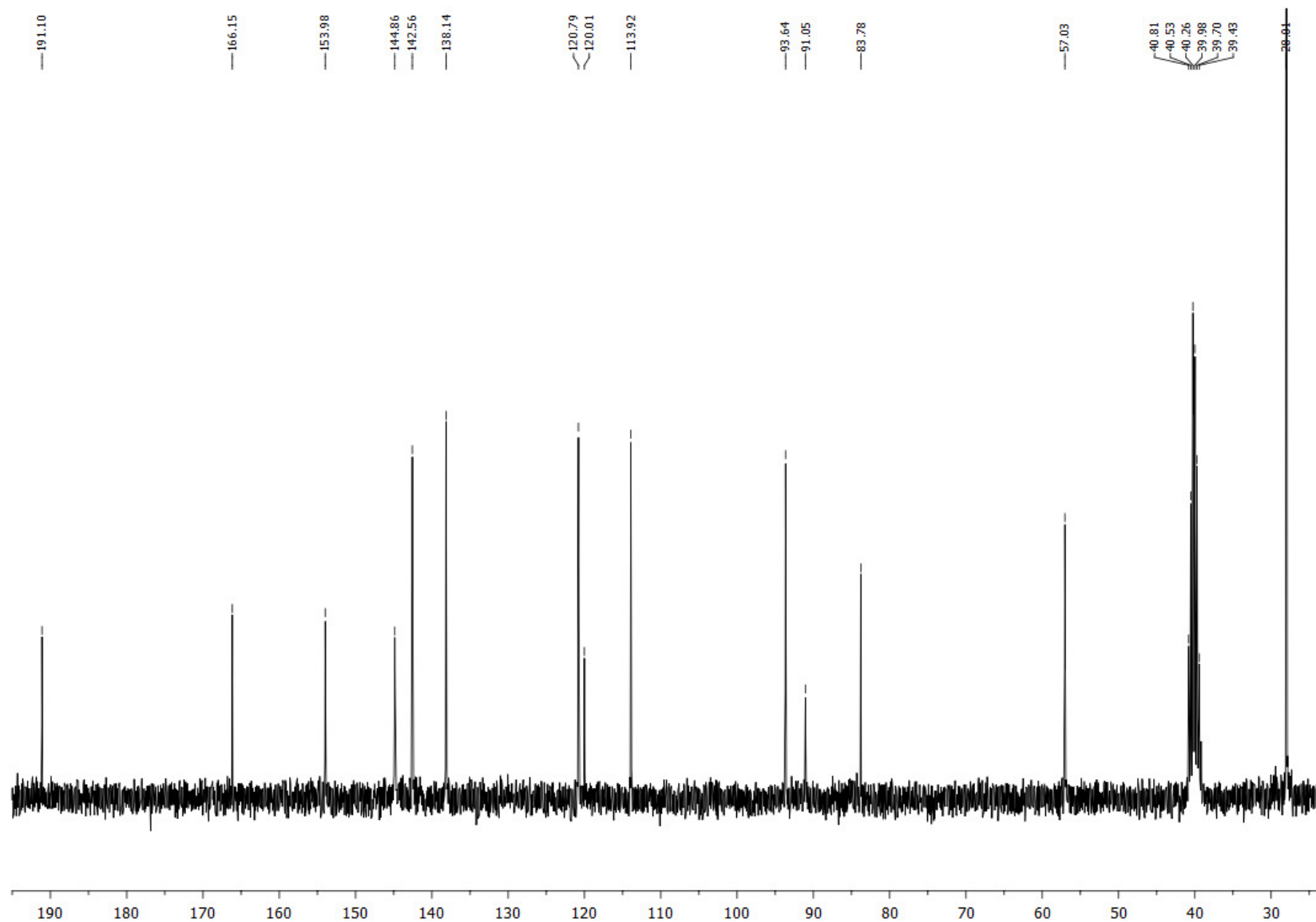
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of ethyl (2E,4E)-4-(1-(2-(*tert*-butoxy)-2-oxoethyl)pyridin-2(1H)-ylidene)-2-cyanobut-2-enoate **6k**



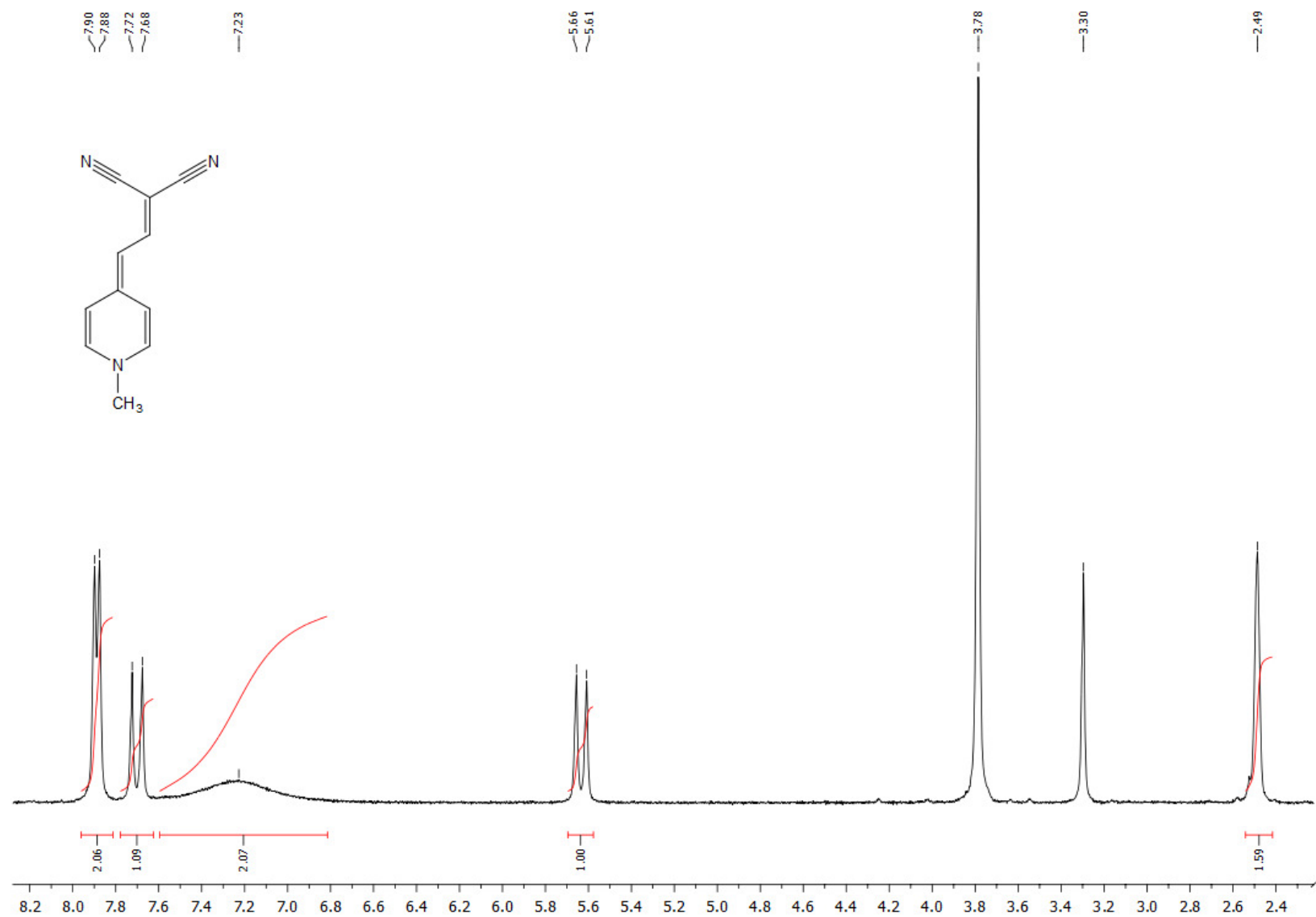
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of ethyl (2E,4E)-4-(1-(2-(*tert*-butoxy)-2-oxoethyl)pyridin-2(1H)-ylidene)-2-cyanobut-2-enoate **6k**



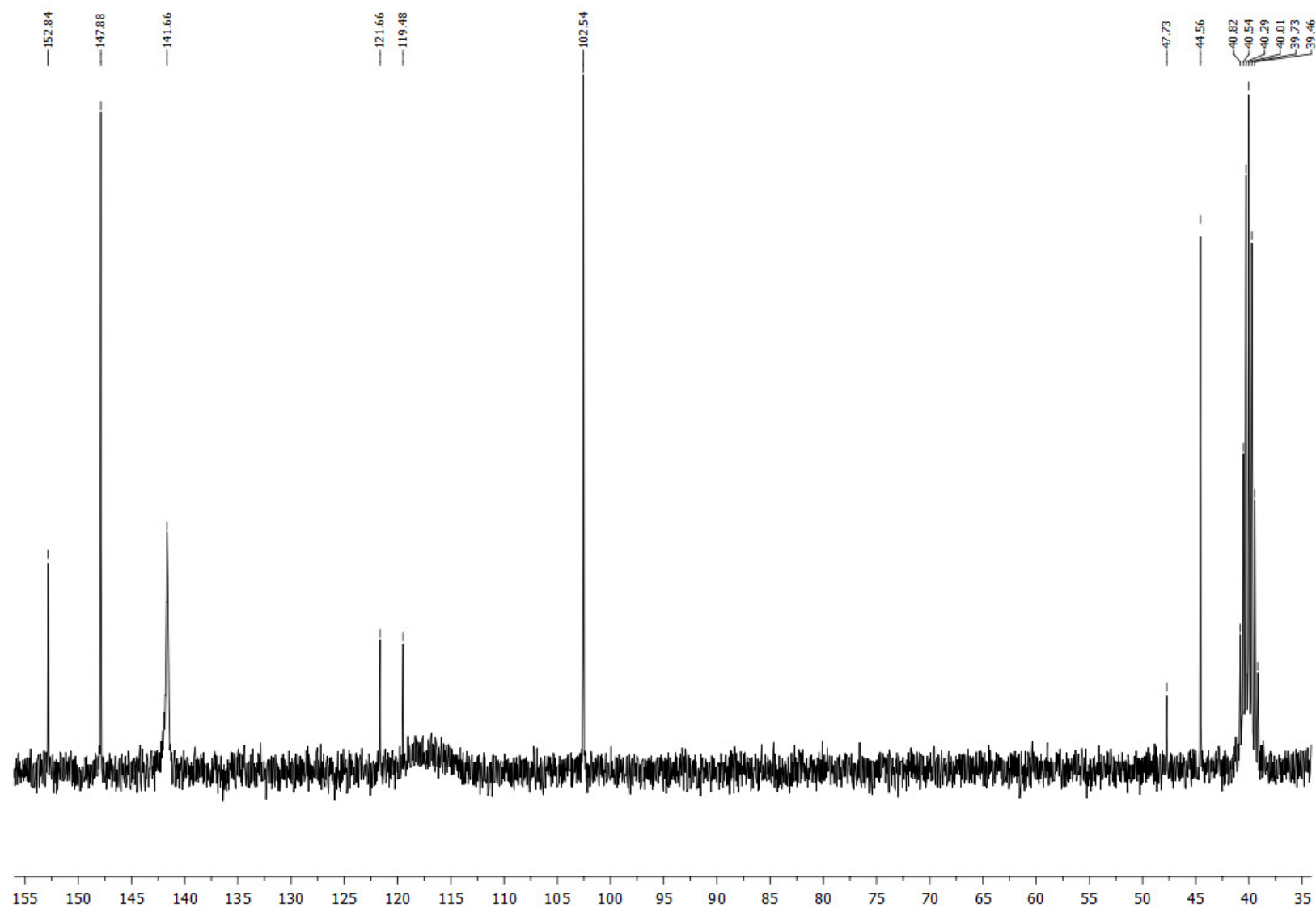
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of *tert*-butyl 2-((*E*)-2-((*E*)-4-amino-3-cyano-4-thioxobut-2-en-1-ylidene)pyridin-1(2H)-yl)acetate **6l**



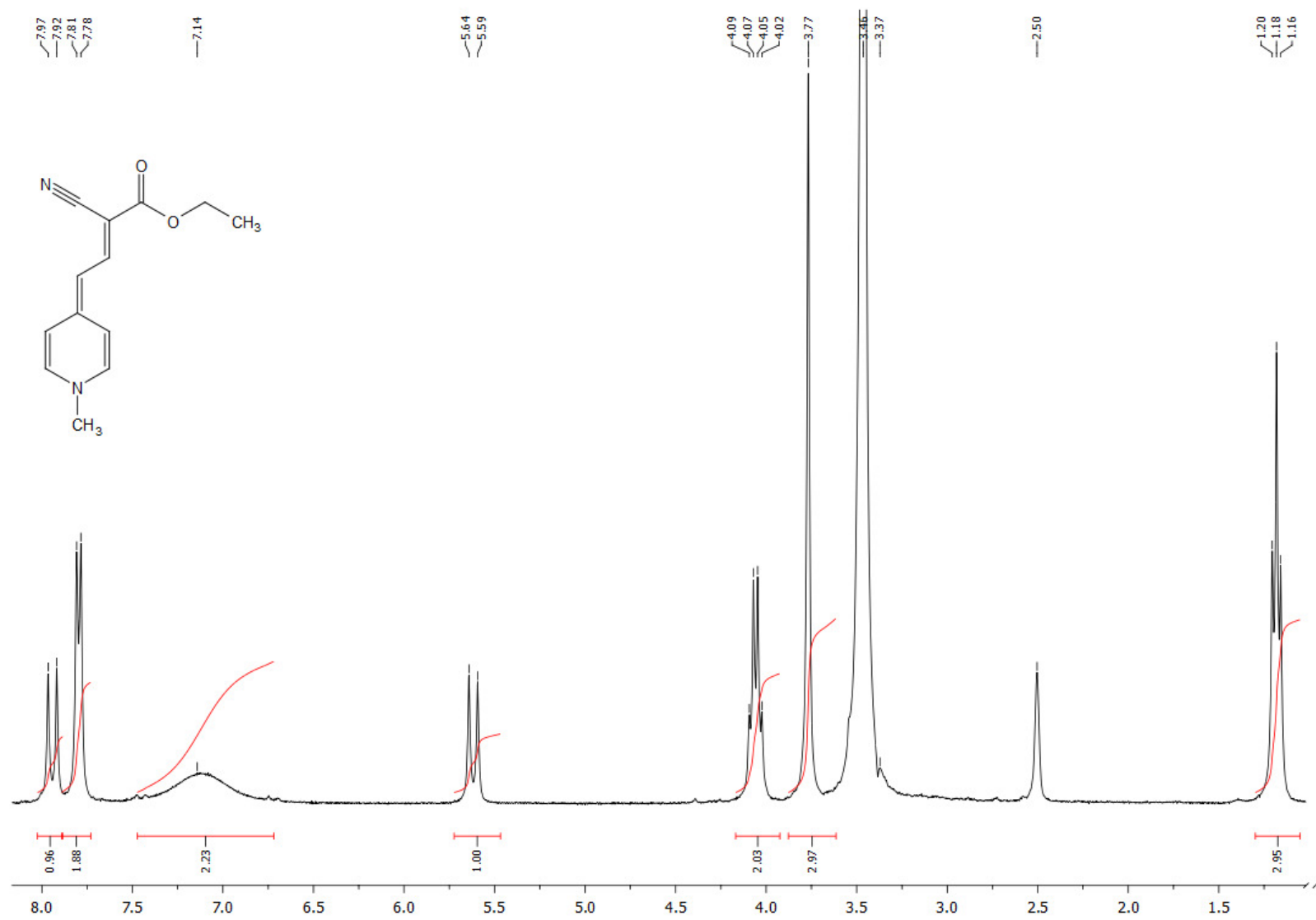
^{13}C NMR (75.5 MHz, $\text{DMSO}-d_6$) spectrum of *tert*-butyl 2-((*E*)-2-((*E*)-4-amino-3-cyano-4-thioxobut-2-en-1-ylidene)pyridin-1(2H)-yl)acetate **6l**



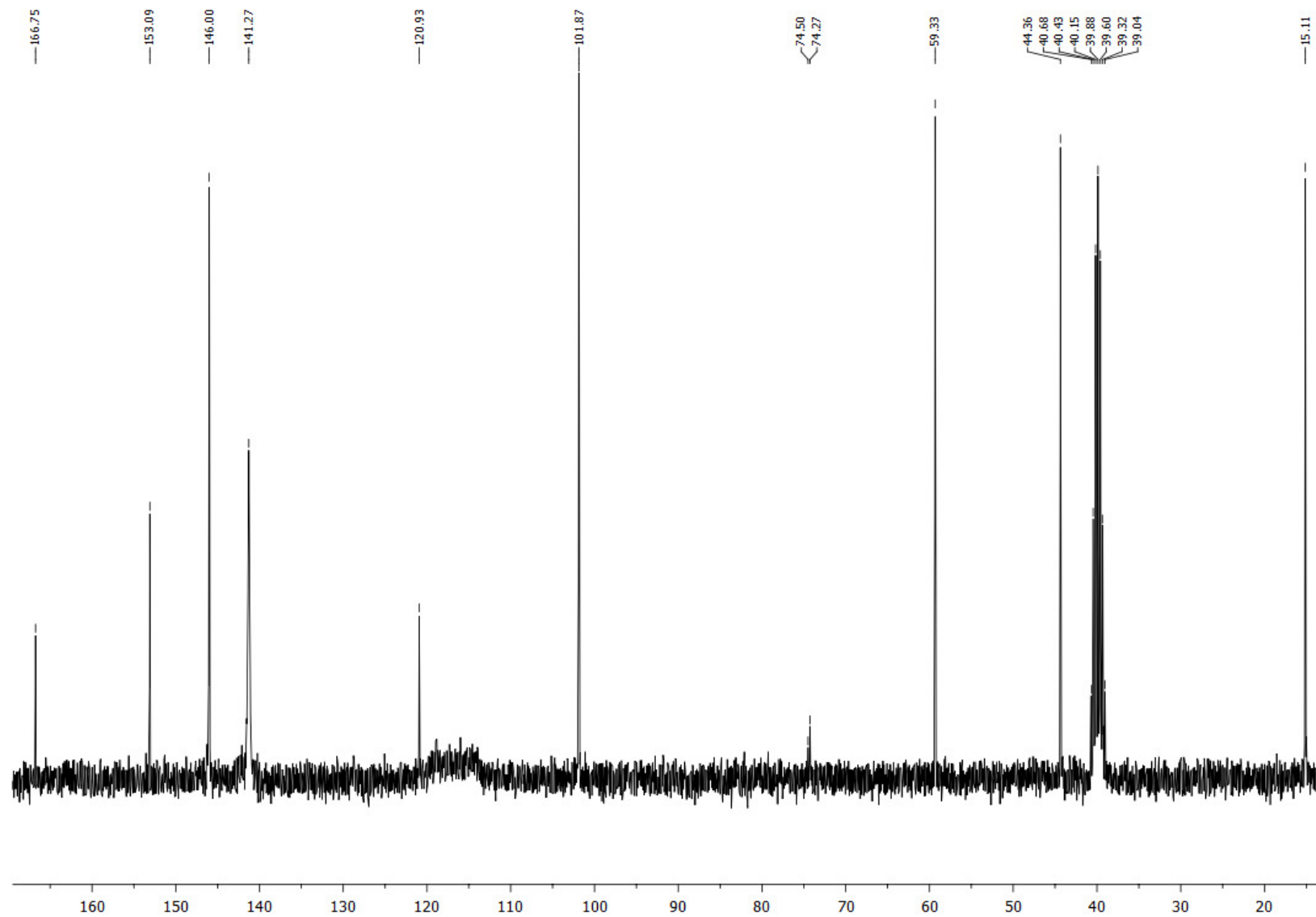
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of 2-(2-(1'-methylpyridin-4'(1*H*)-ylidene)ethylidene)malononitrile **7a**



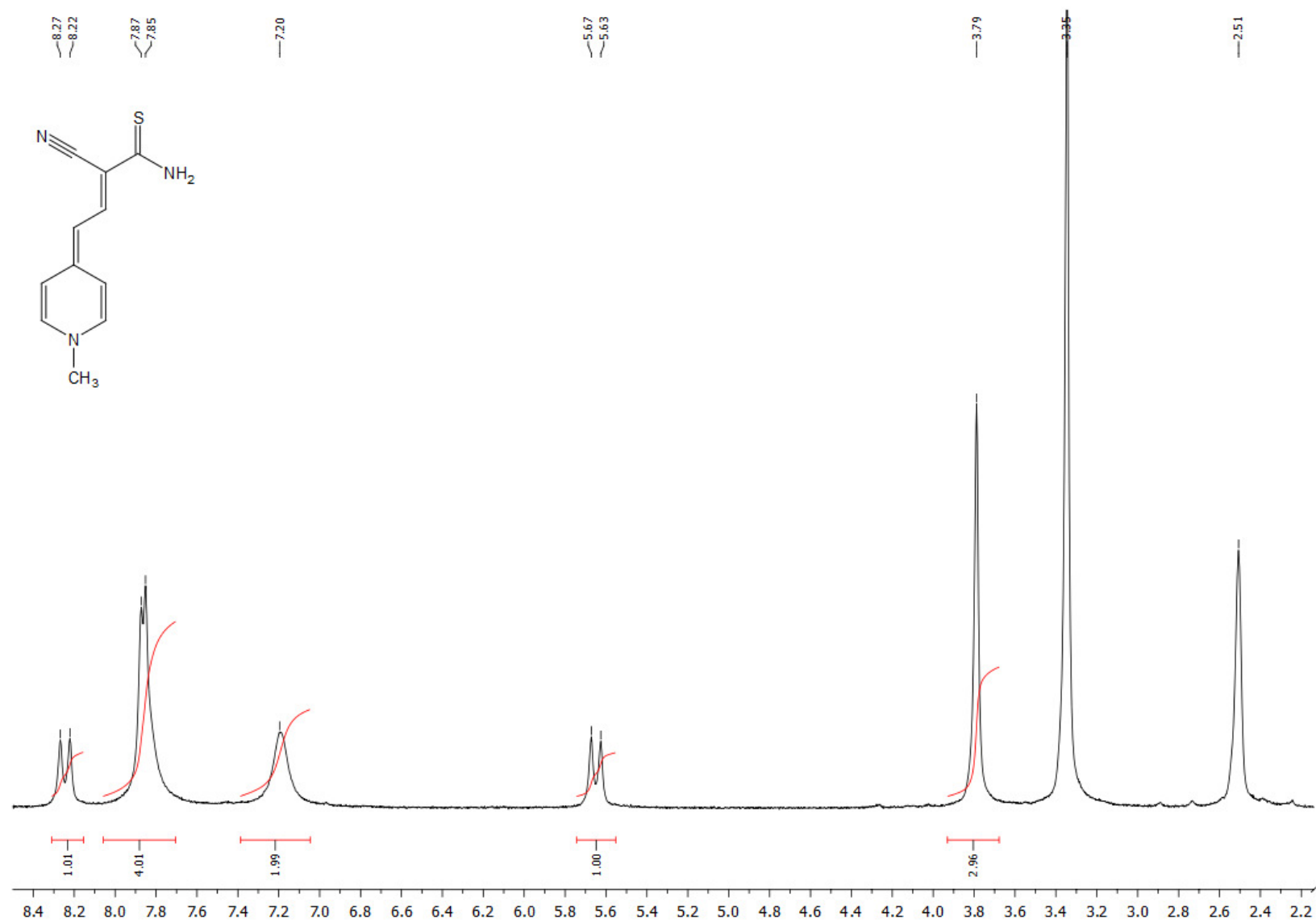
^{13}C NMR (75.5 MHz, $\text{DMSO}-d_6$) spectrum of 2-(2-(1'-methylpyridin-4'(1*H*)-ylidene)ethylidene)malononitrile **7a**



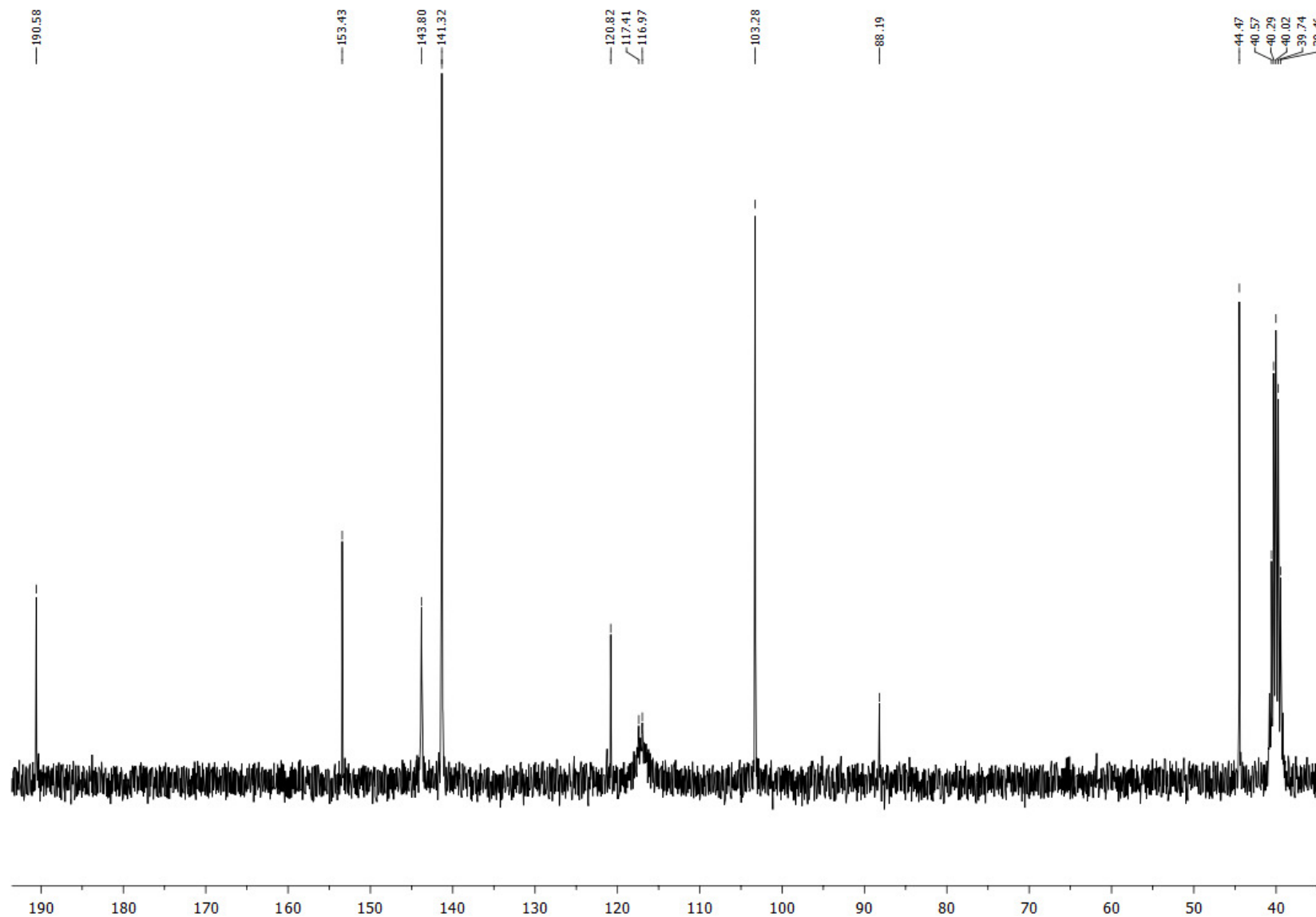
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of ethyl (Z)-2-cyano-4-(1'-methylpyridin-4'(1'*H*)-ylidene)but-2-enoate **7b**



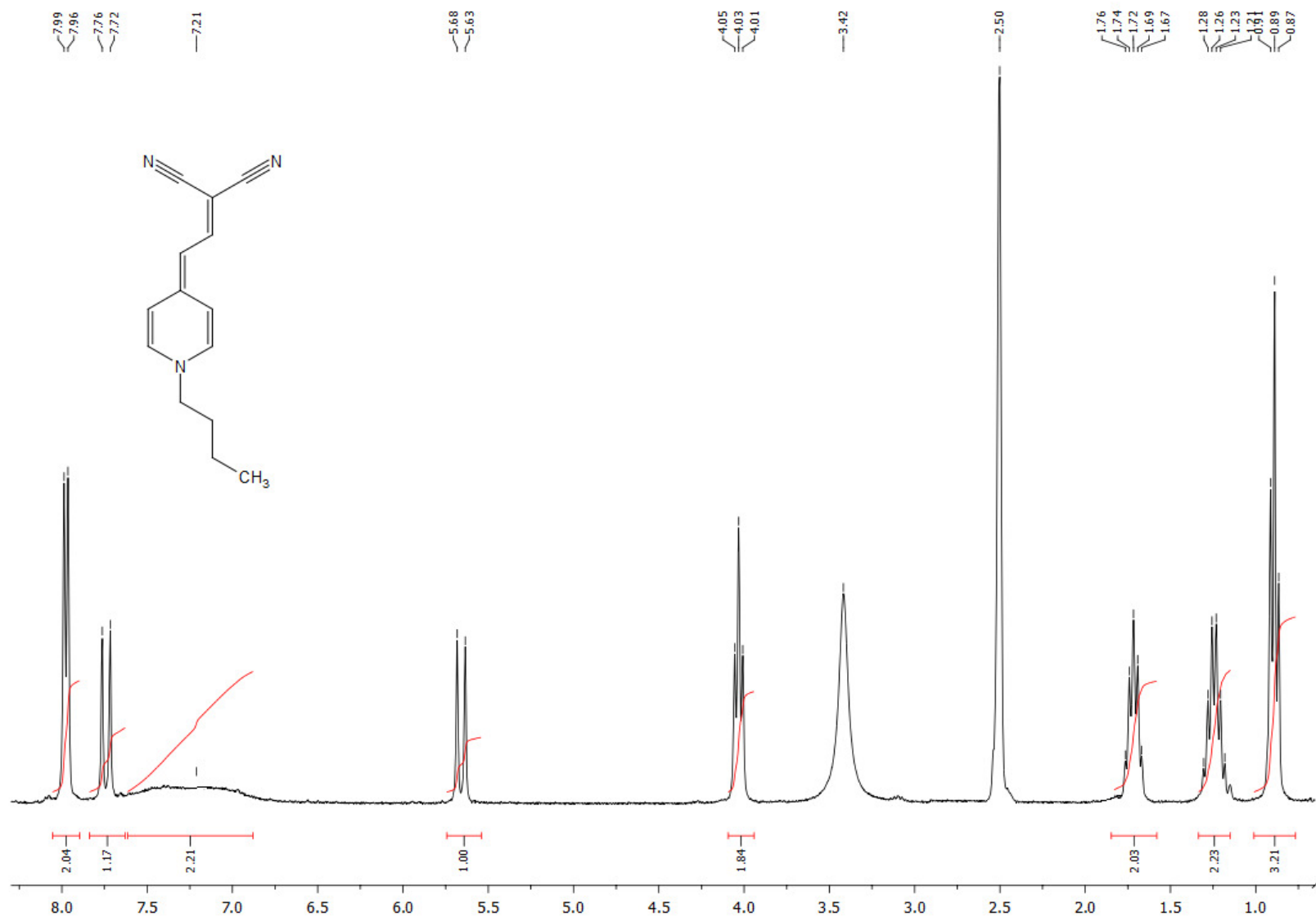
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of ethyl (Z)-2-cyano-4-(1'-methylpyridin-4'(1'H)-ylidene)but-2-enoate **7b**



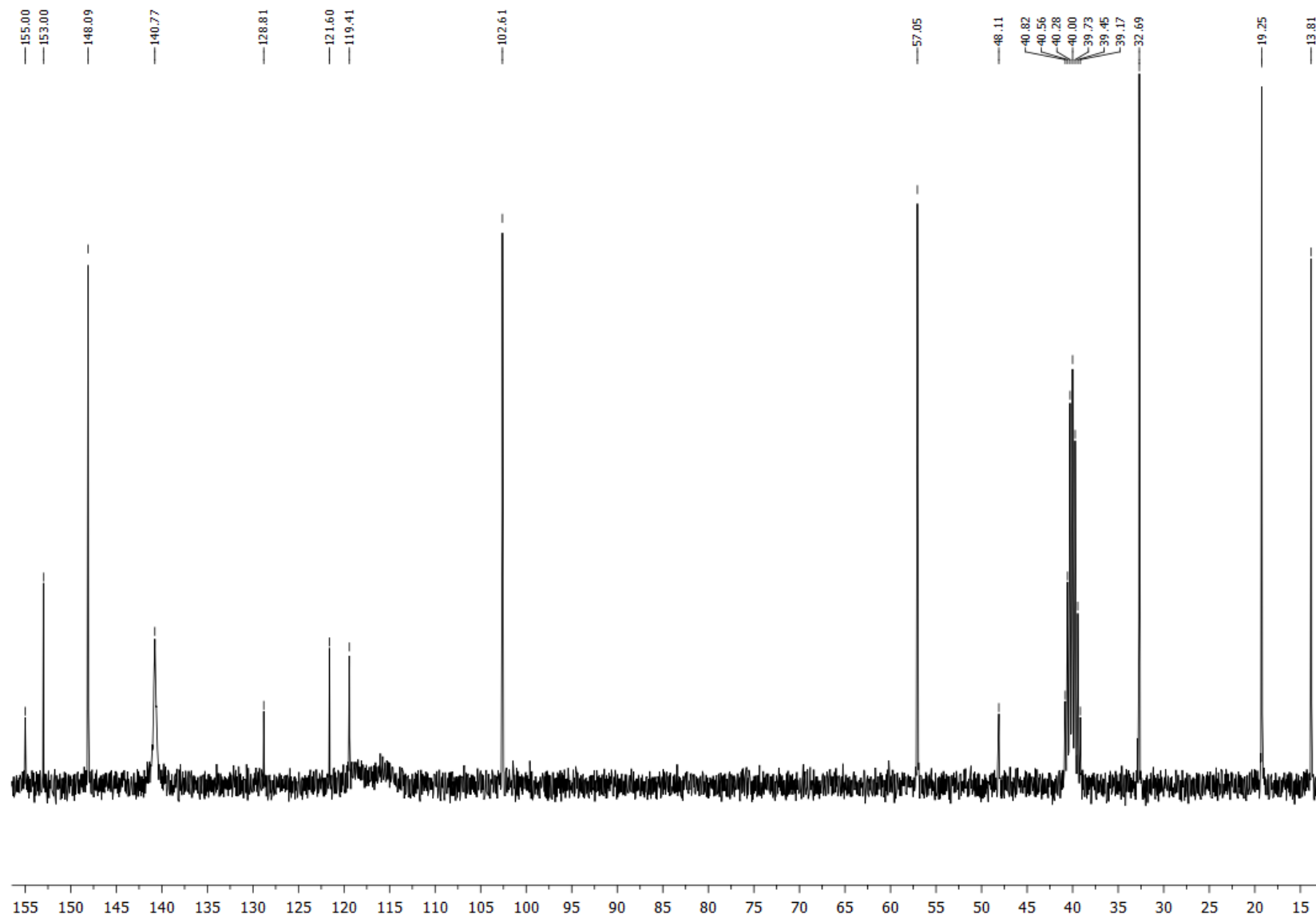
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of (Z)-2-cyano-4-(1'-methylpyridin-4'(1'*H*)-ylidene)but-2-enethioamide **7c**



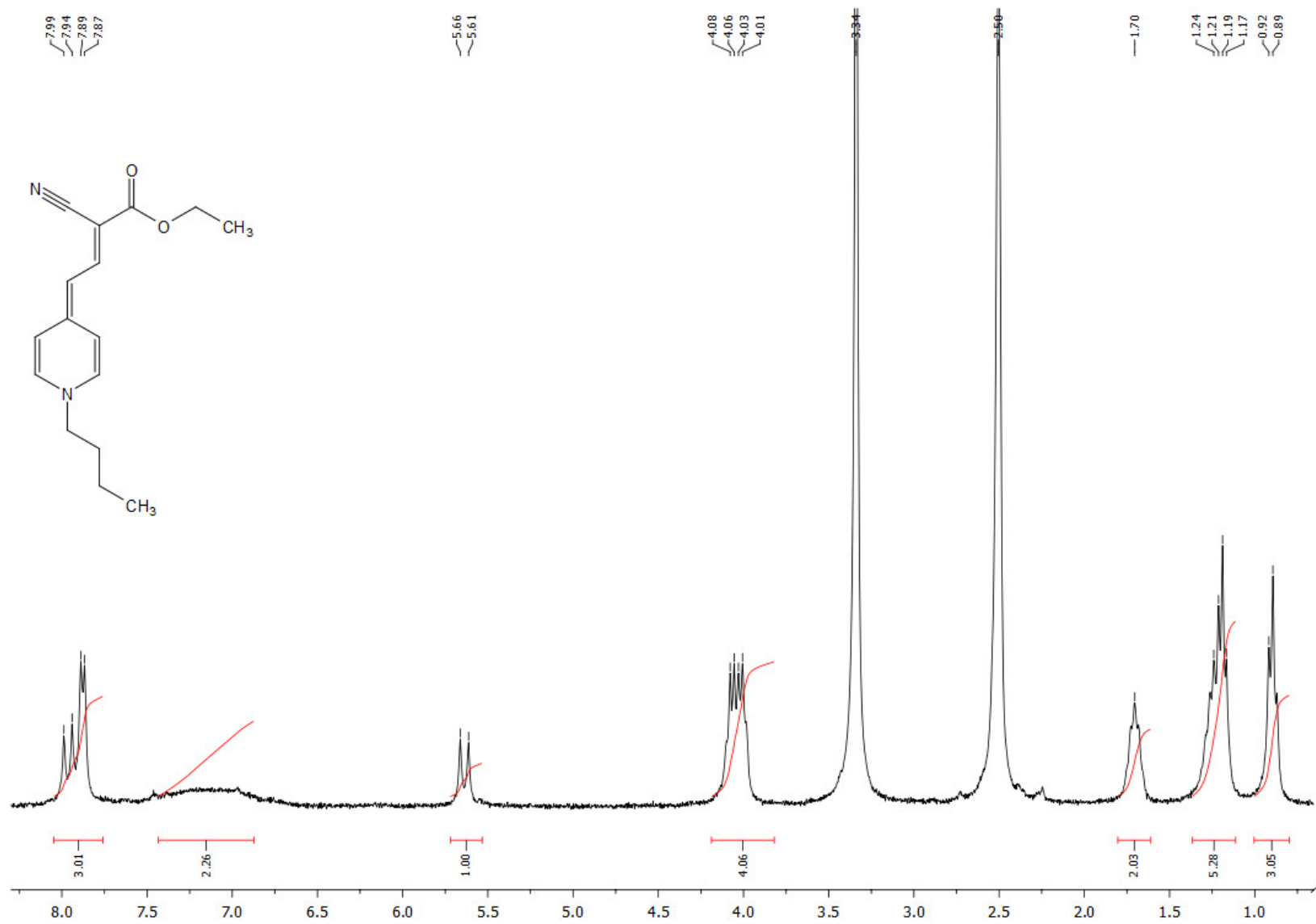
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of (Z)-2-cyano-4-(1'-methylpyridin-4'(1'H)-ylidene)but-2-enethioamide **7c**



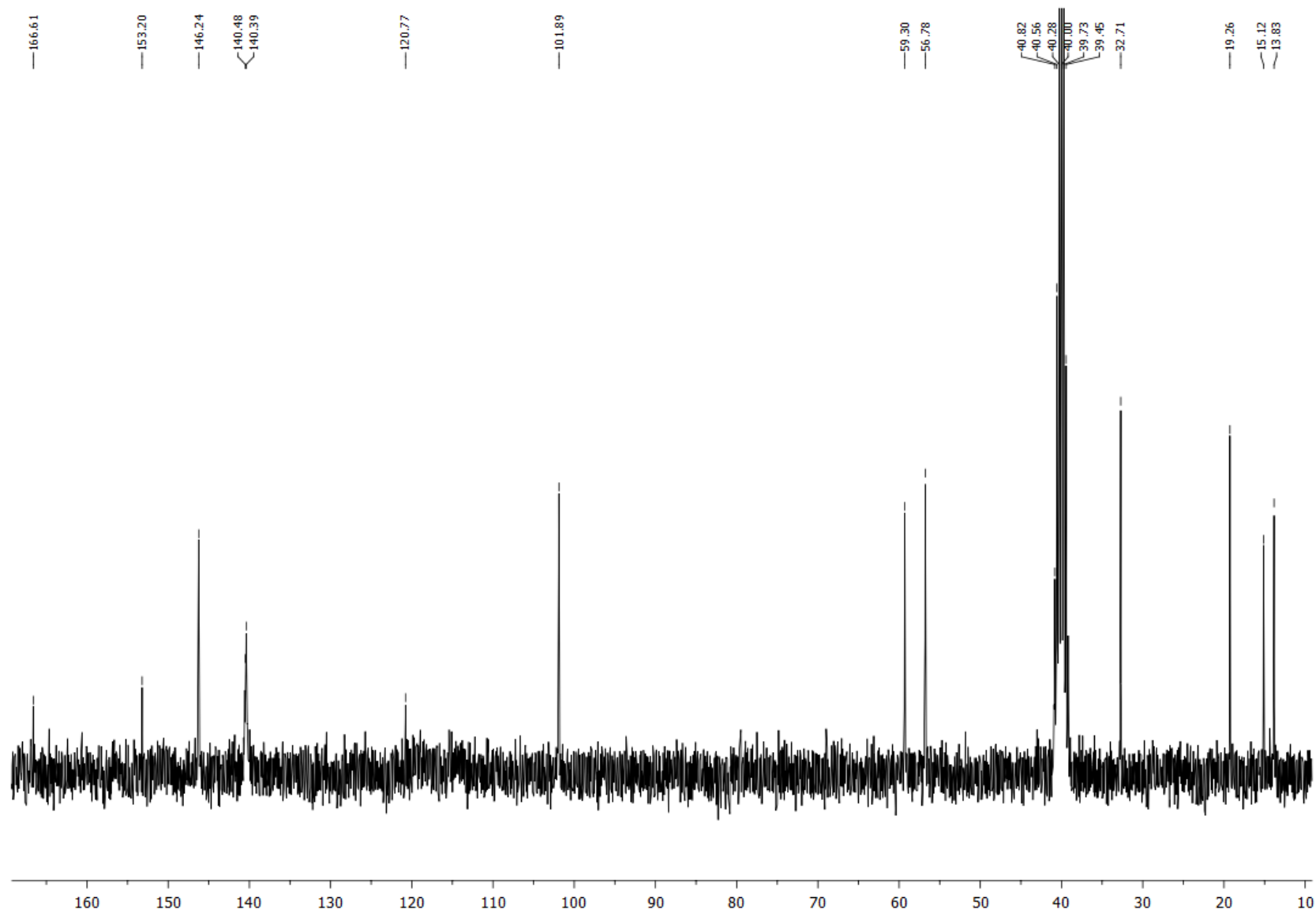
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of 2-(2-(1'-butylpyridin-4'(1H)-ylidene)ethylidene)malononitrile **7d**



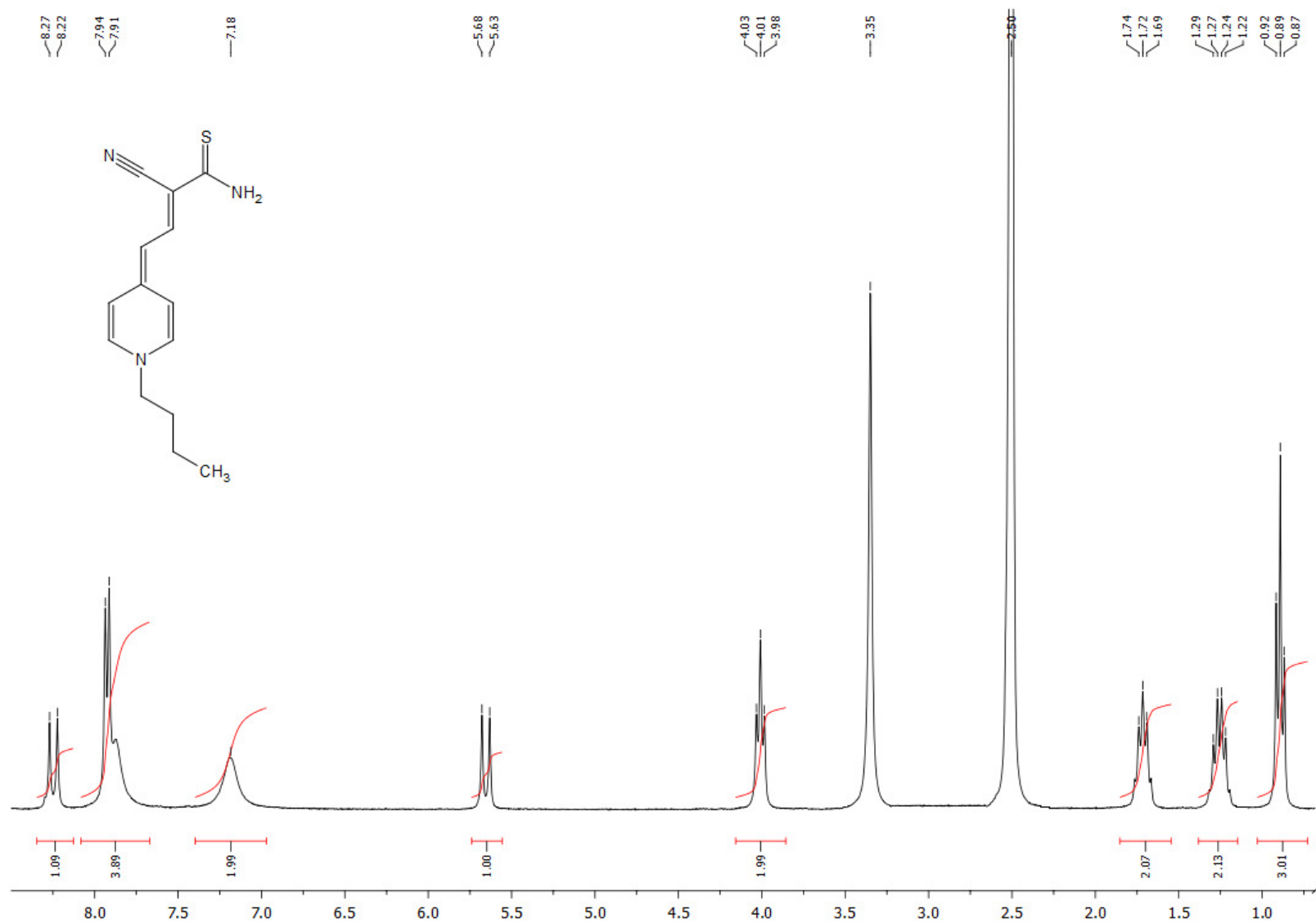
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of 2-(2-(1'-butylpyridin-4'(1'*H*)-ylidene)ethylidene)malononitrile **7d**



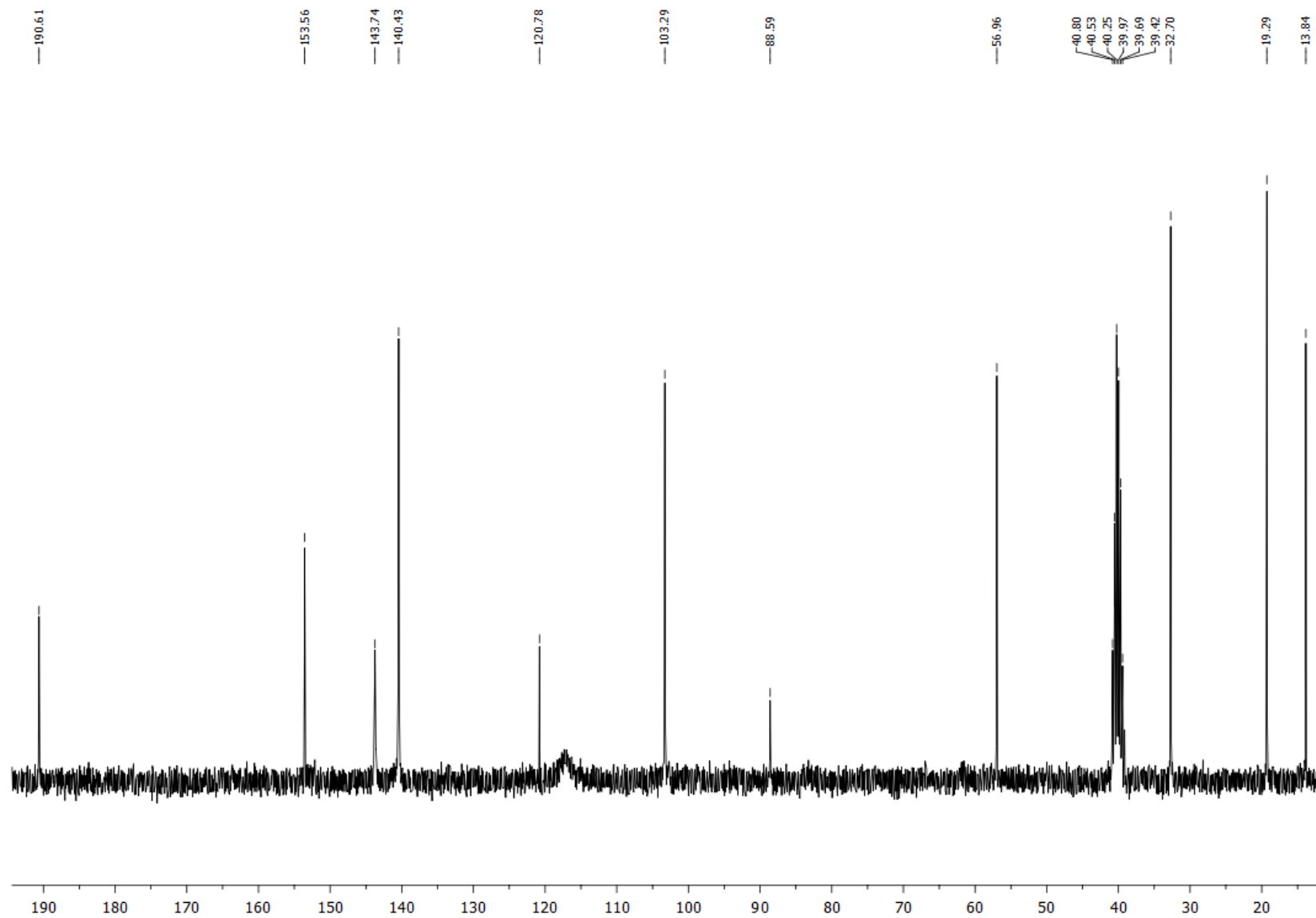
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of ethyl (Z)-2-cyano-4-(1-butylpyridin-4(1H)-ylidene)but-2-enoate **7e**



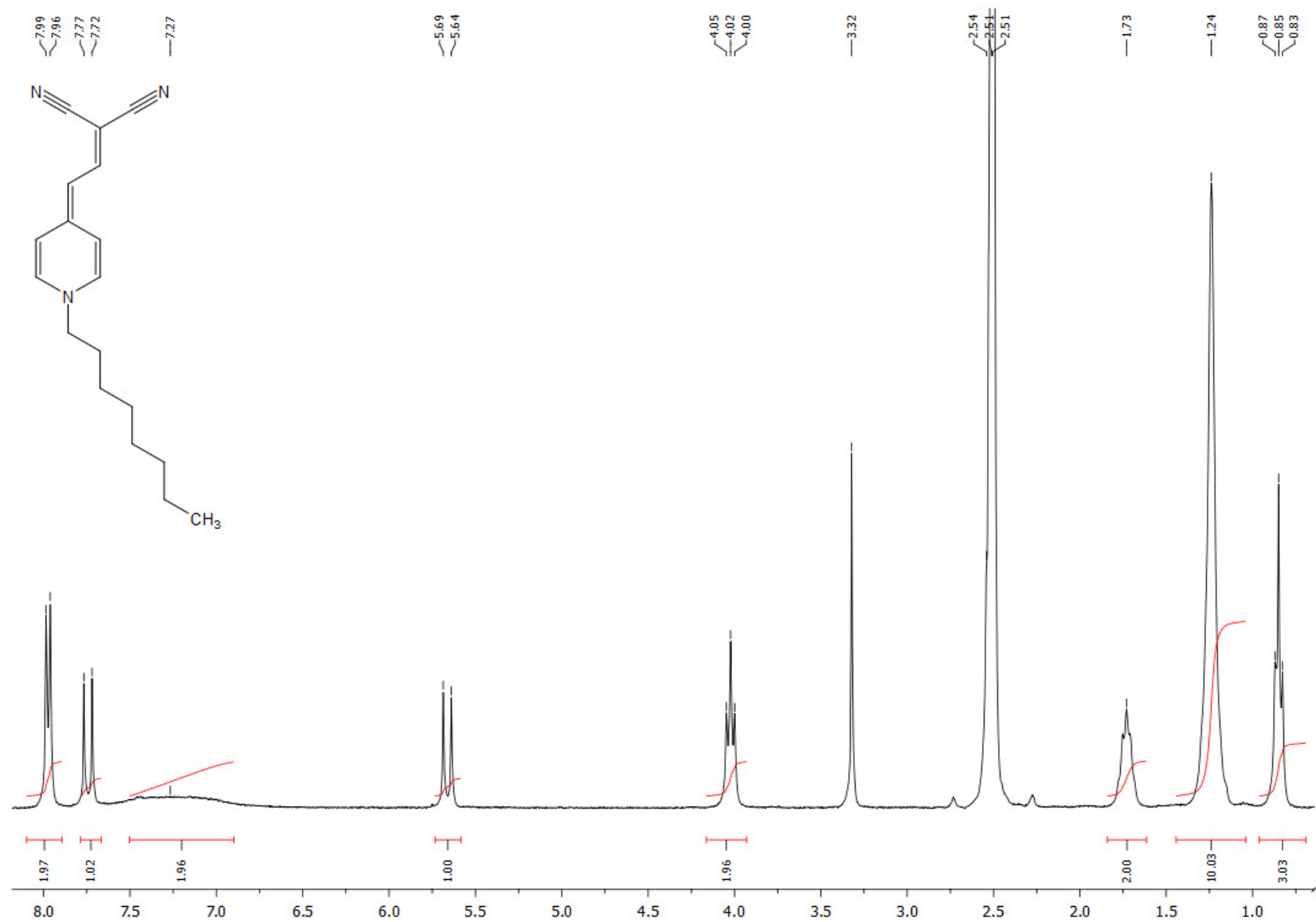
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of ethyl (Z)-2-cyano-4-(1-butylpyridin-4(1H)-ylidene)but-2-enoate **7e**



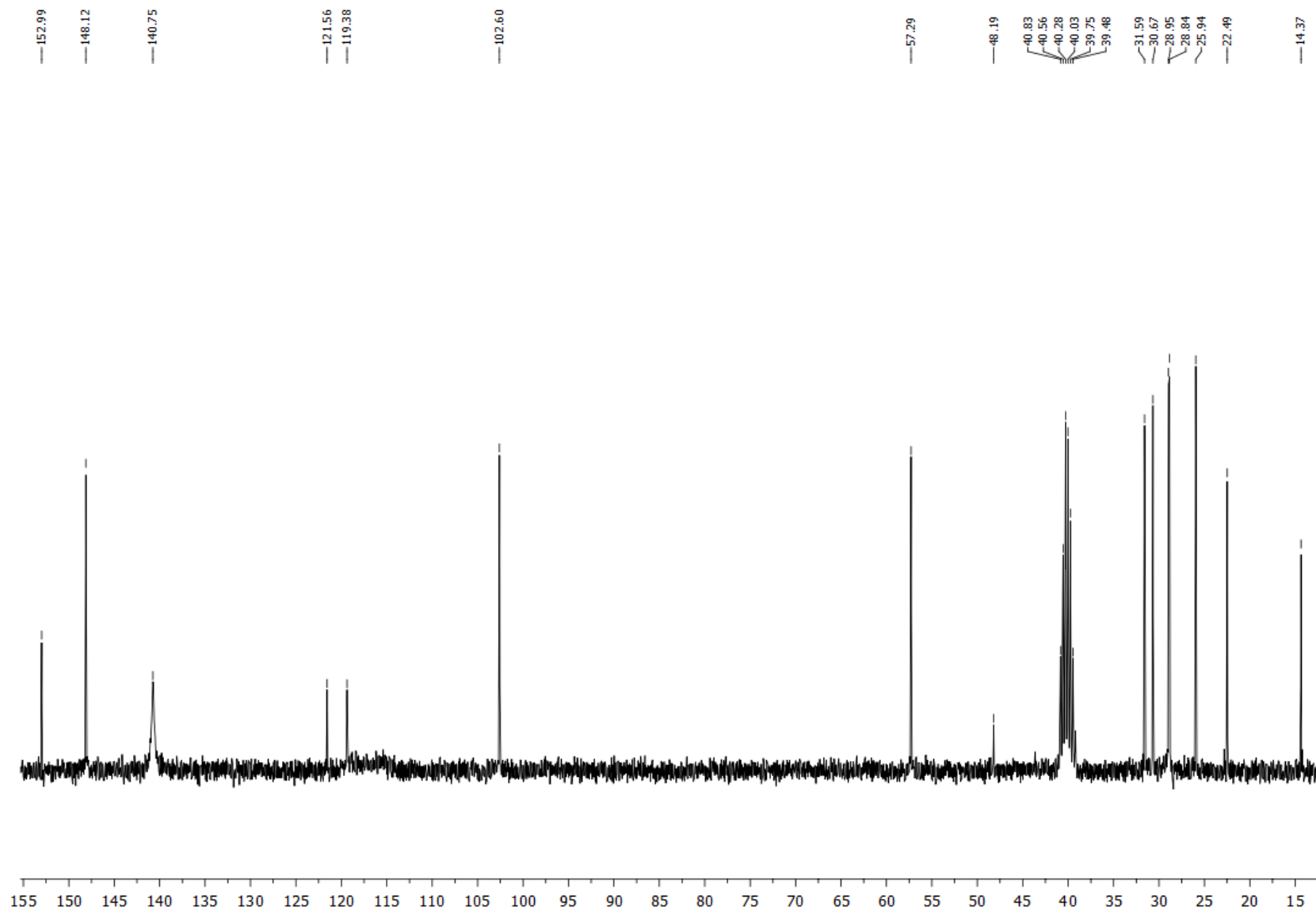
¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of (Z)-2-cyano-4-(1'-butylpyridin-4'(1'H)-ylidene)but-2-enethioamide **7f**



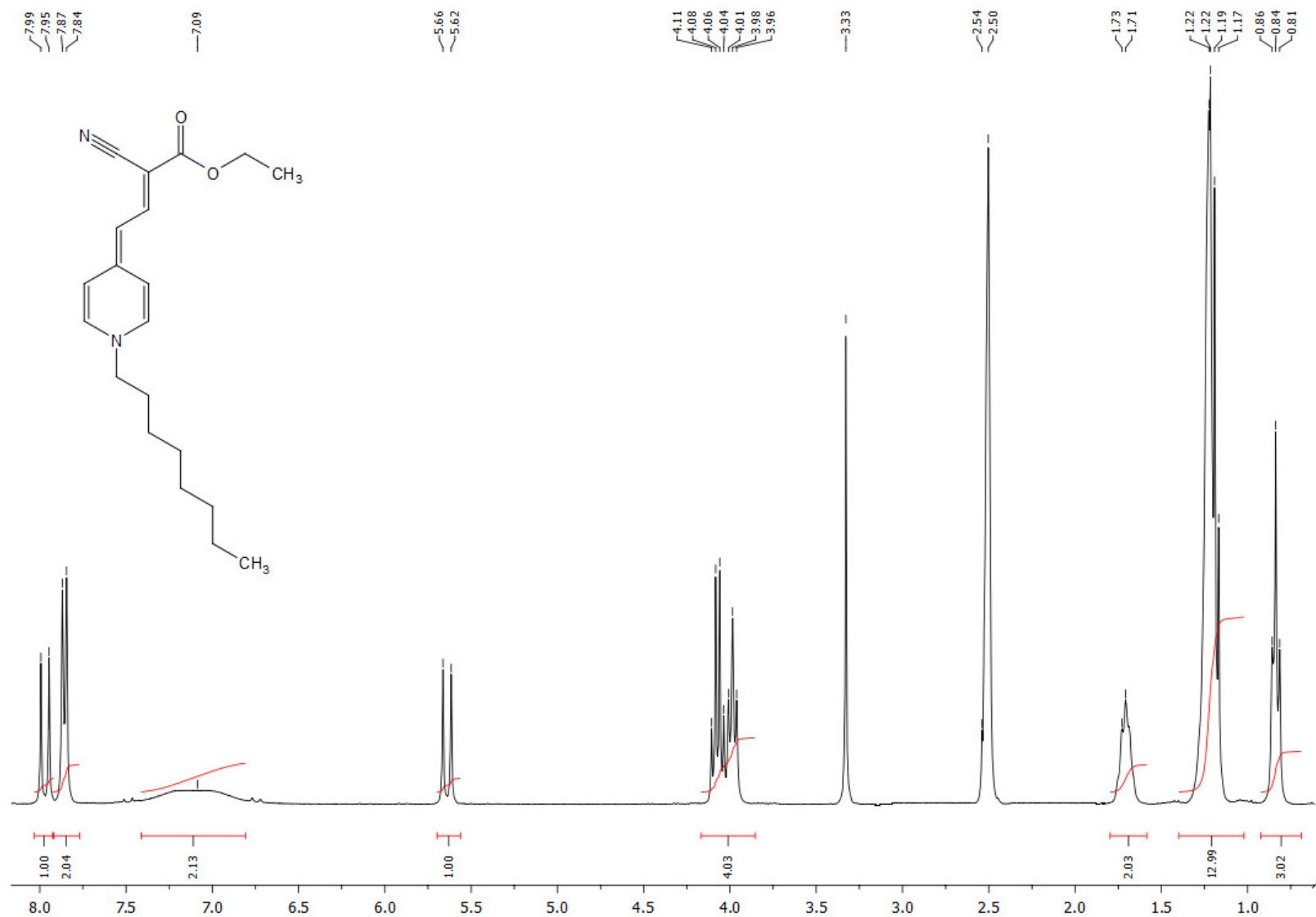
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of (Z)-2-cyano-4-(1'-butylpyridin-4'(1'H)-ylidene)but-2-enethioamide **7f**



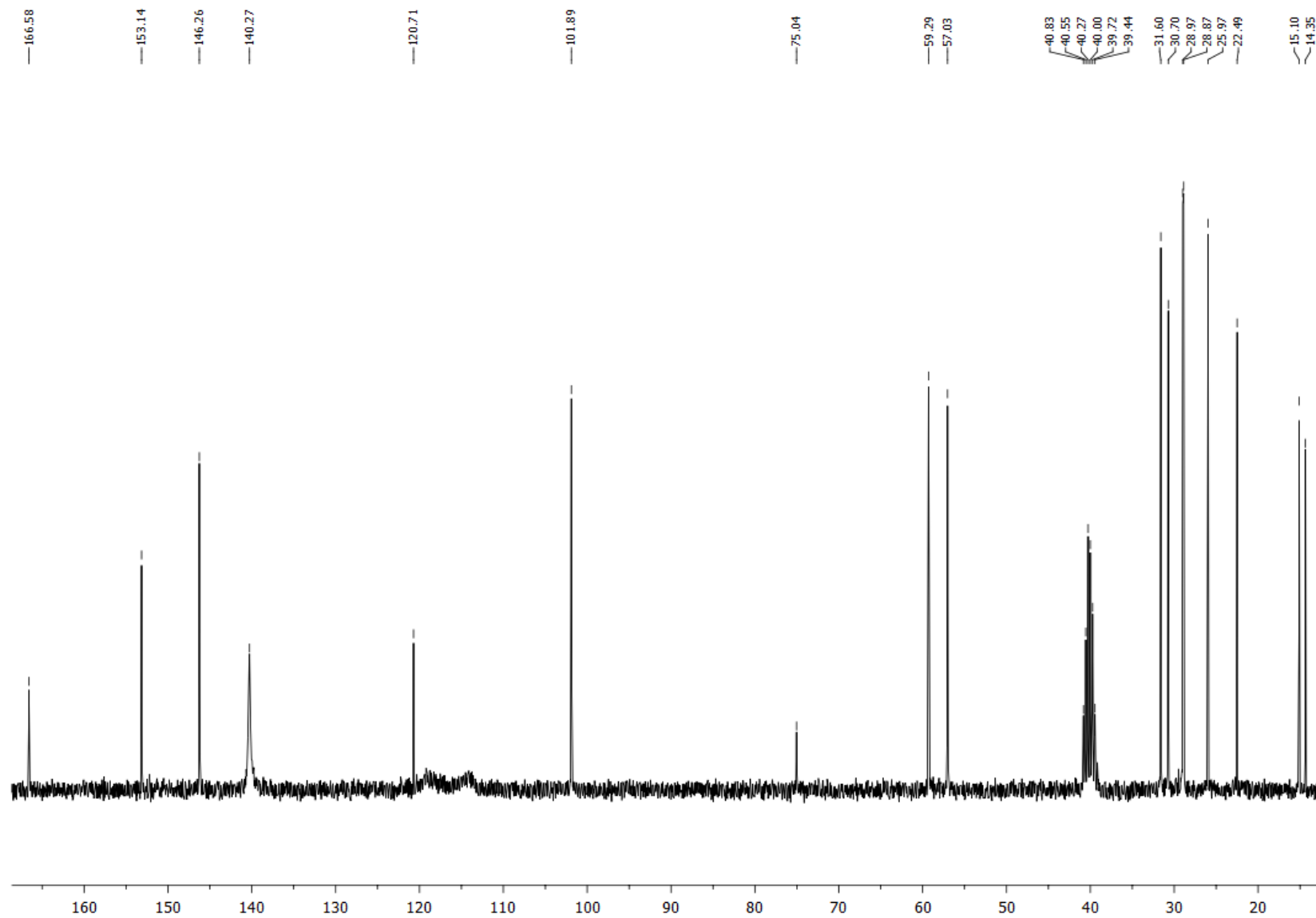
^1H NMR (300.1 MHz, $\text{DMSO}-d_6$) spectrum of 2-(2-(1'-octylpyridin-4'(1'H)-ylidene)ethylidene)malononitrile **7g**



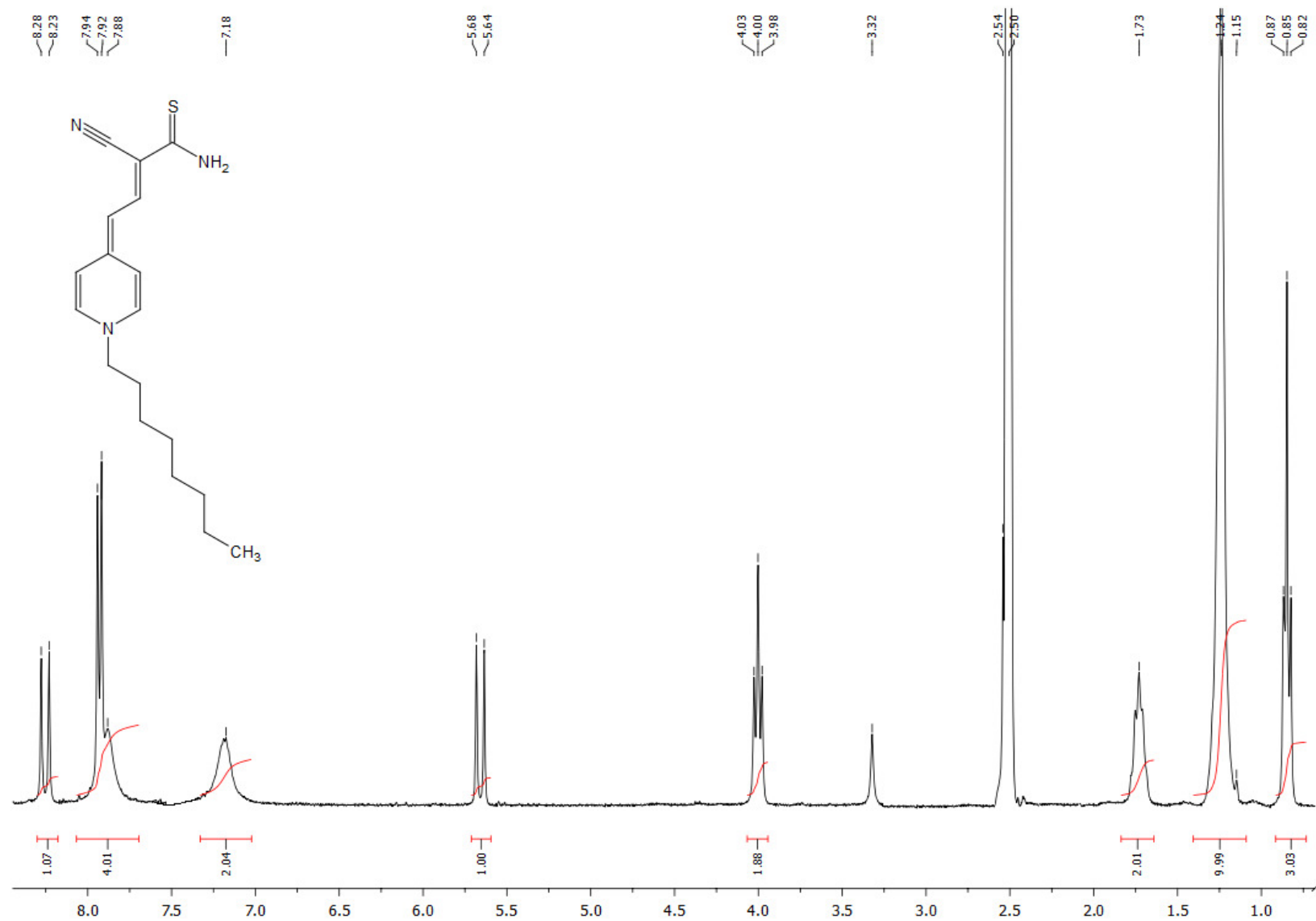
^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of 2-(2-(1'-octylpyridin-4'(1'*H*)-ylidene)ethylidene)malononitrile **7g**



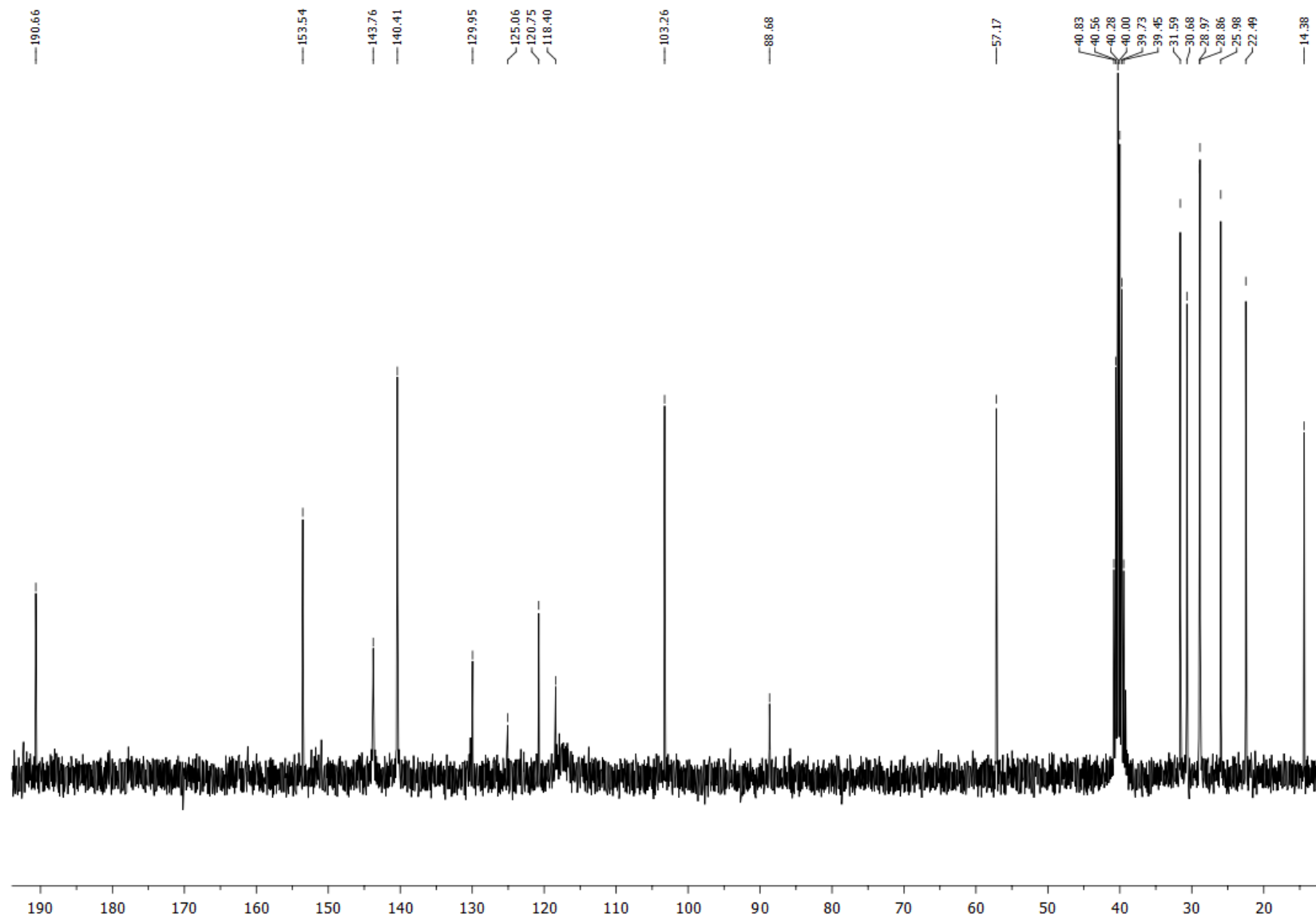
^1H NMR (300.1 MHz, $\text{DMSO-}d_6$) spectrum of ethyl (Z)-2-cyano-4-(1'-octylpyridin-4'(1'H)-ylidene)but-2-enoate **7h**



^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) spectrum of ethyl (Z)-2-cyano-4-(1'-octylpyridin-4'(1H)-ylidene)but-2-enoate **7h**



¹H NMR (300.1 MHz, DMSO-*d*₆) spectrum of (Z)-2-cyano-4-(1-octylpyridin-4(1H)-ylidene)but-2-enethioamide **7i**



^{13}C NMR (75.5 MHz, $\text{DMSO}-d_6$) spectrum of (Z)-2-cyano-4-(1-octylpyridin-4(1H)-ylidene)but-2-enethioamide **7i**

Copies of NMR Spectra for 2-(3,3-dicyanoallyl)-1-methylpyridin-1-ium 2,2,2-trifluoroacetate **6a.1**