

Guanidine Functionalized Anthranilamides as Effective Antibacterials with Biofilm Disruption Activity

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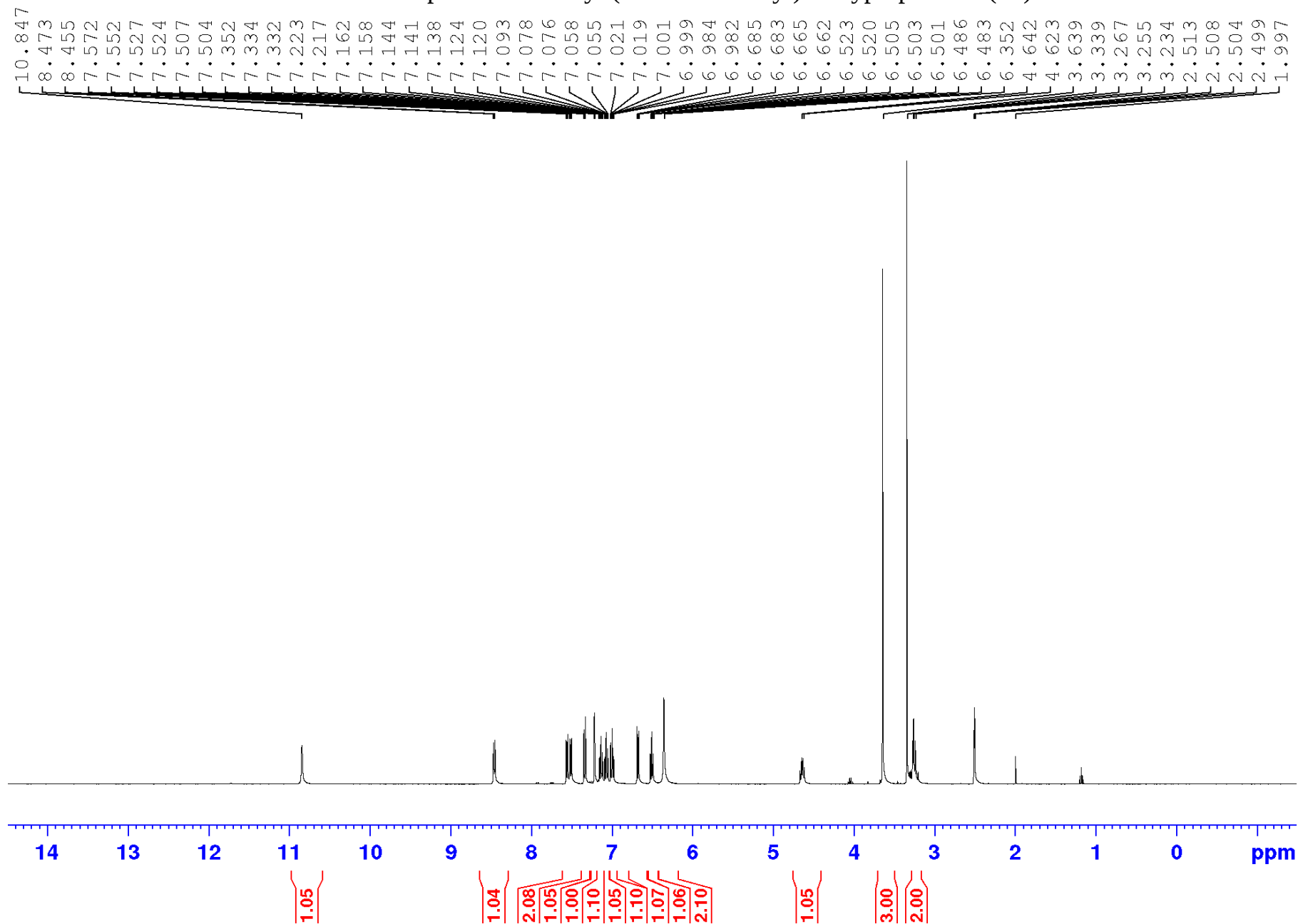
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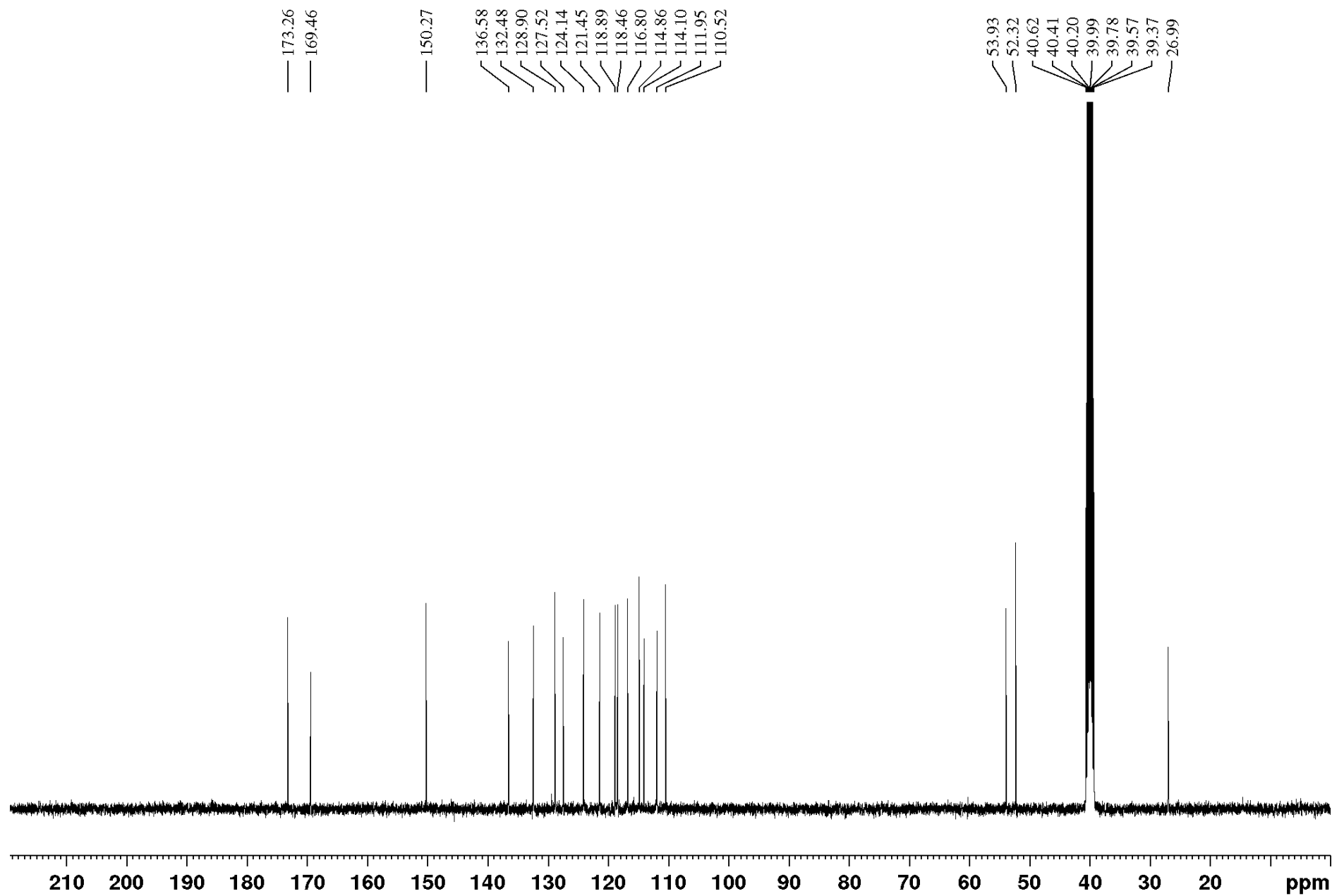
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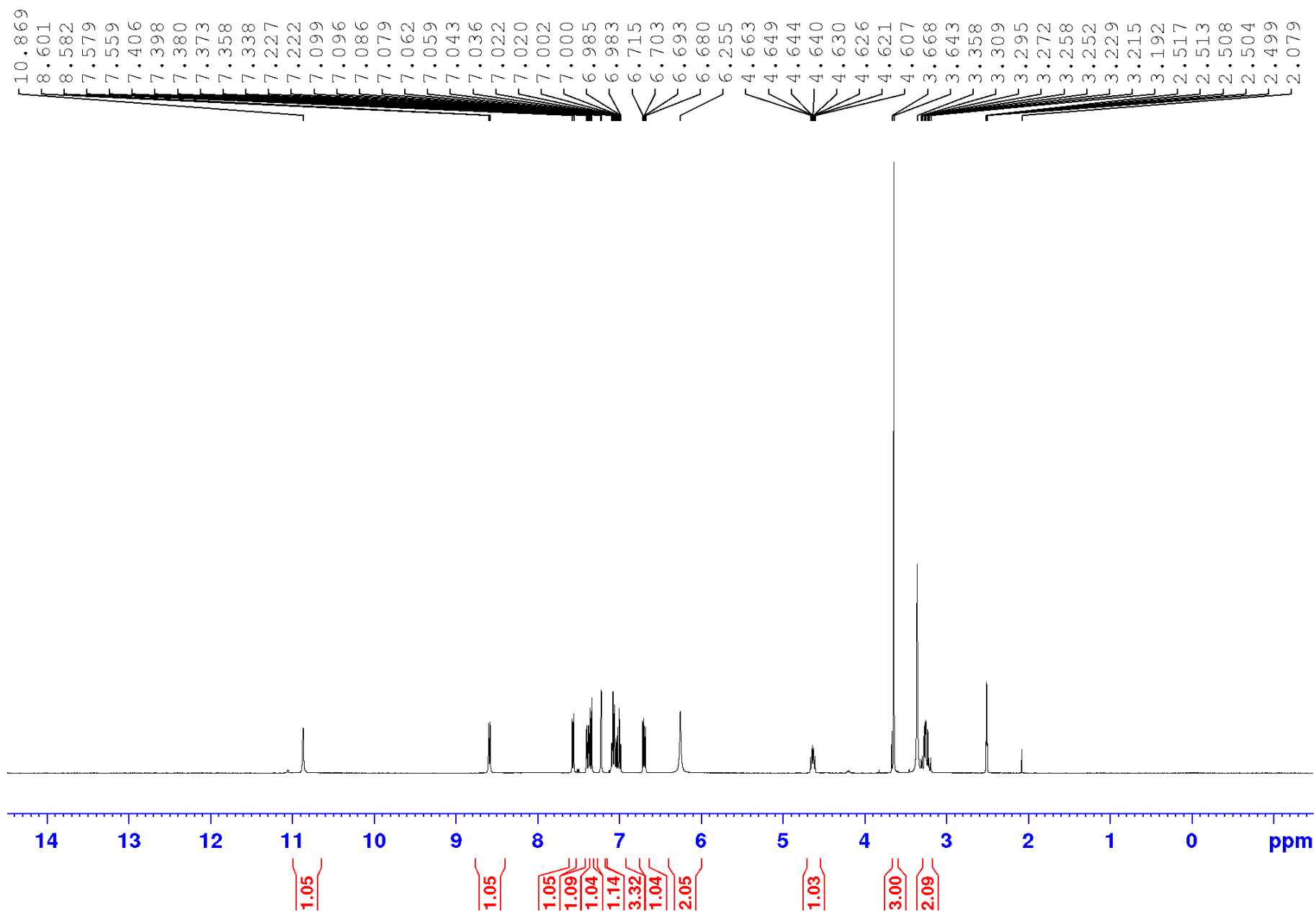
¹H NMR spectra of Methyl (2-aminobenzoyl)-L-tryptophanate (2a)



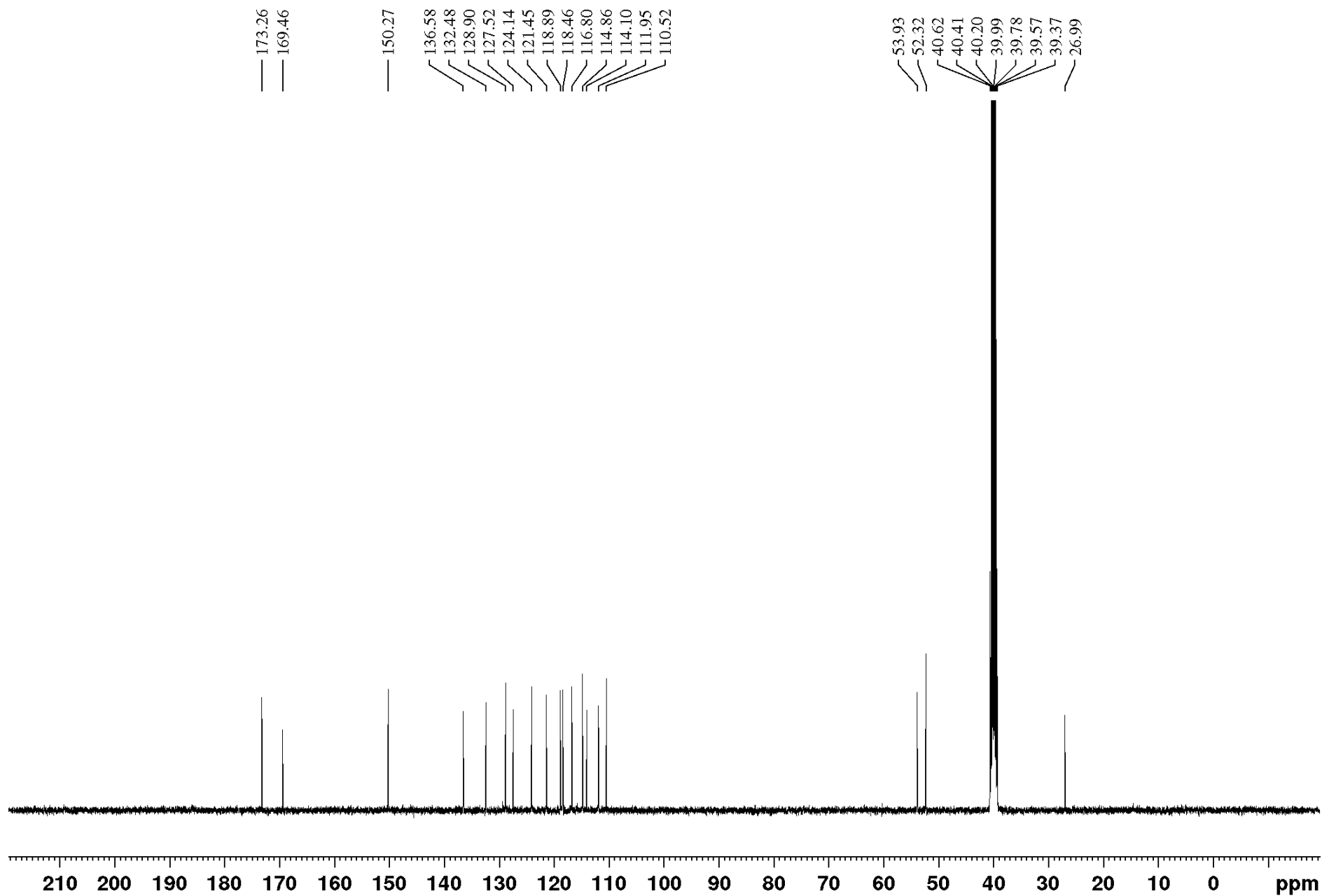
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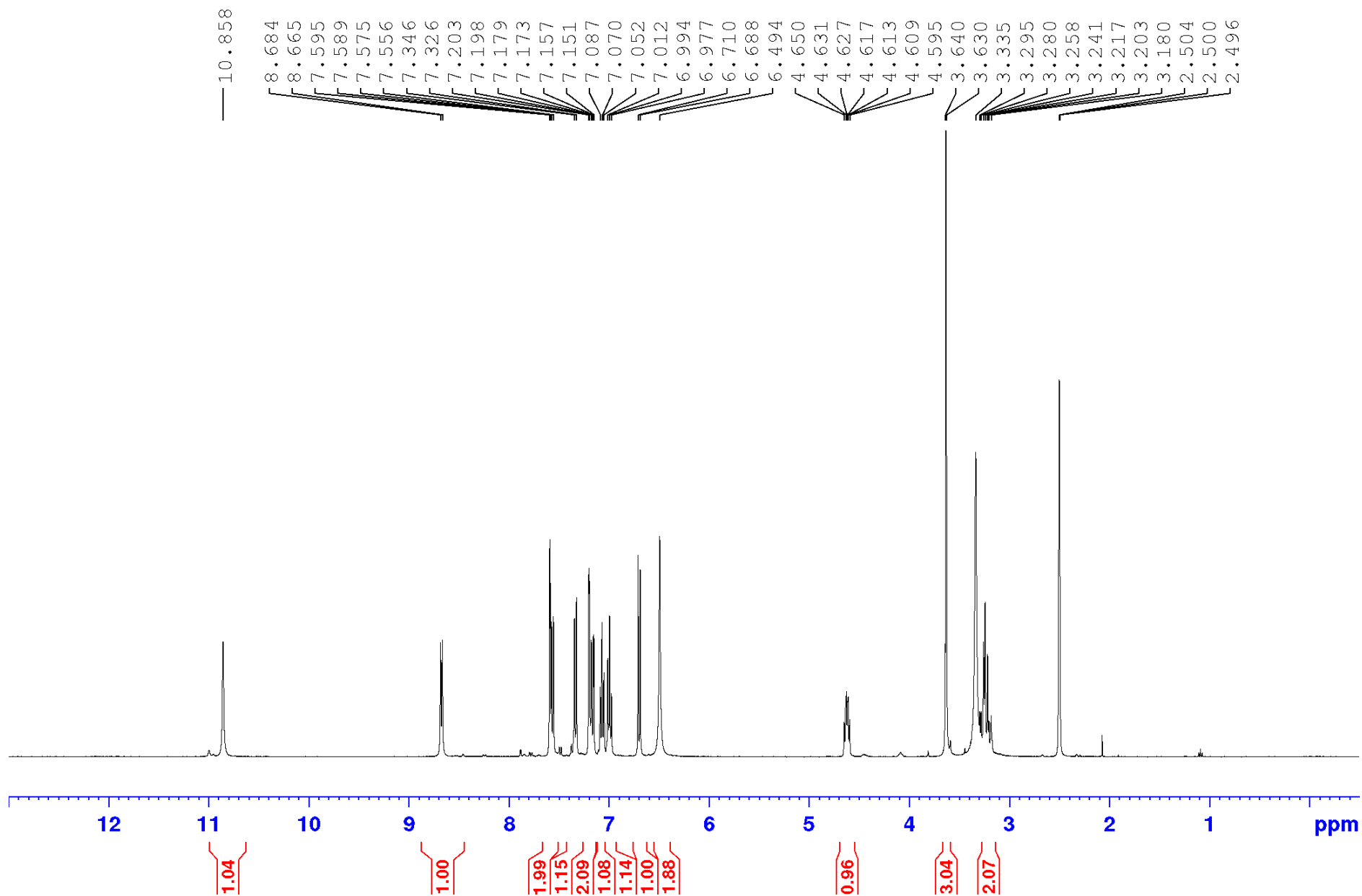
¹H NMR spectra of Methyl (2-amino-5-fluorobenzoyl)-*L*-tryptophanate (**2b**)



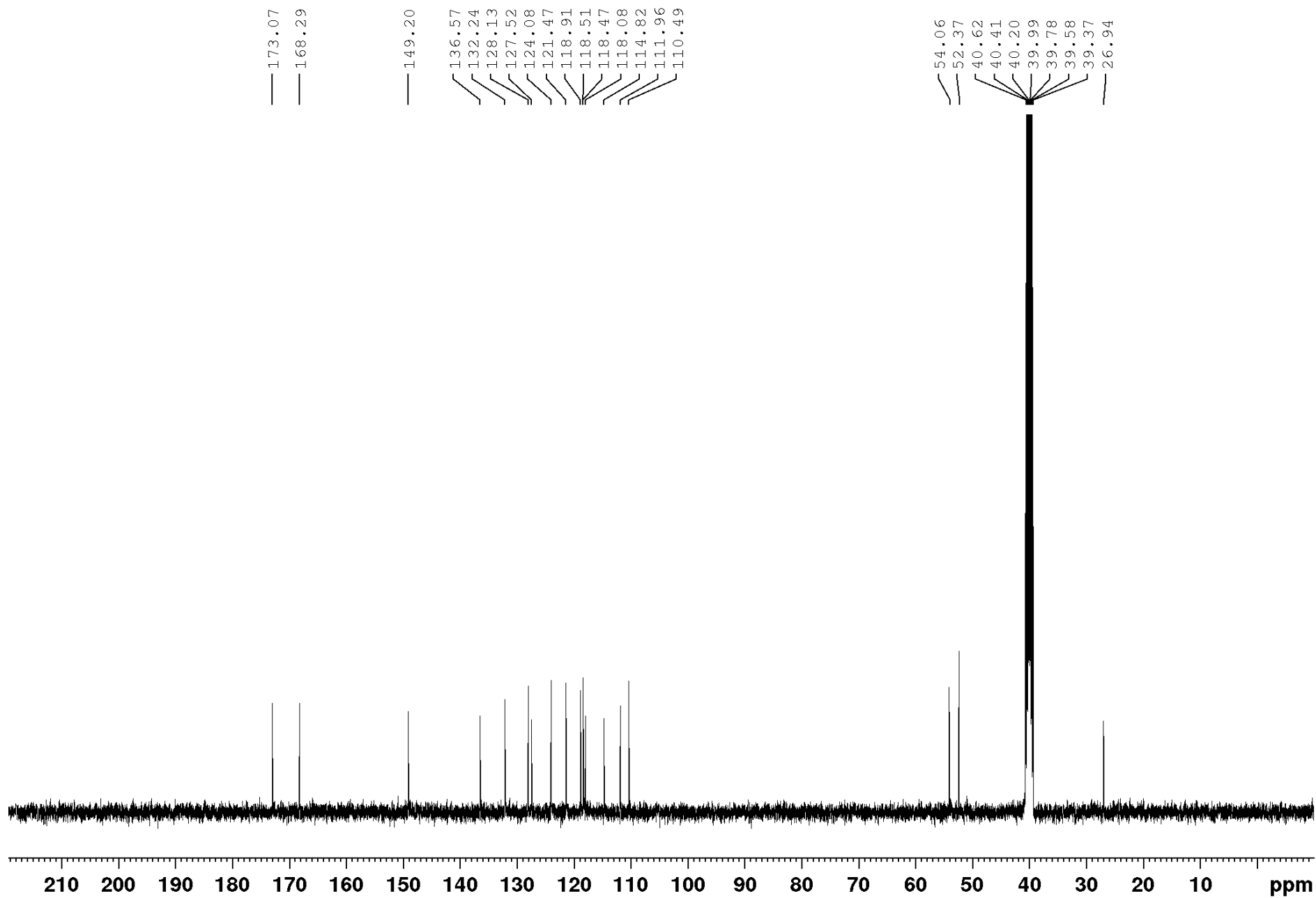
^{13}C NMR spectra of Methyl (2-amino-5-fluorobenzoyl)-*L*-tryptophanate (**2b**)



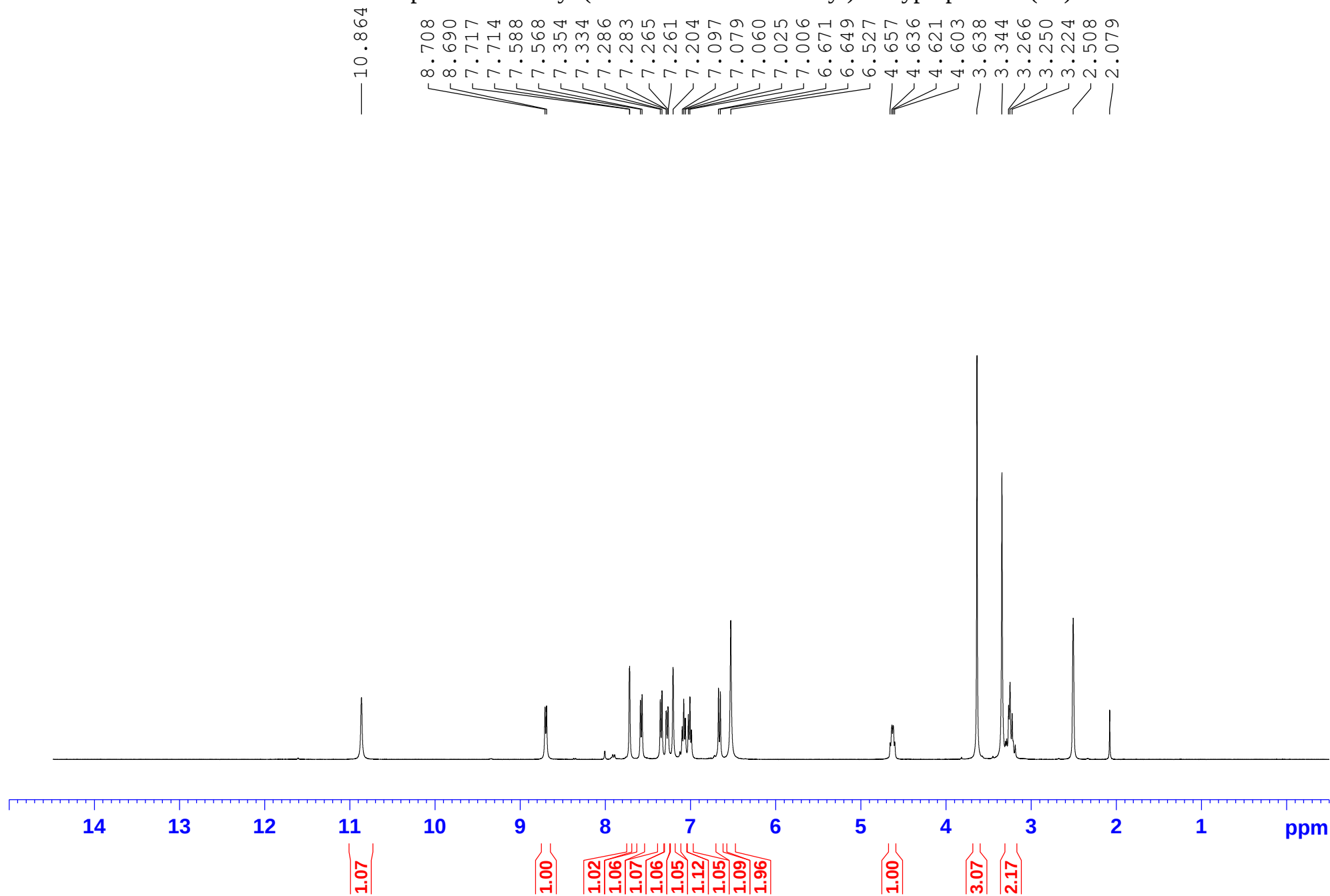
¹H NMR spectra of Methyl (2-amino-5-chlorobenzoyl)-*L*-tryptophanate (**2c**)



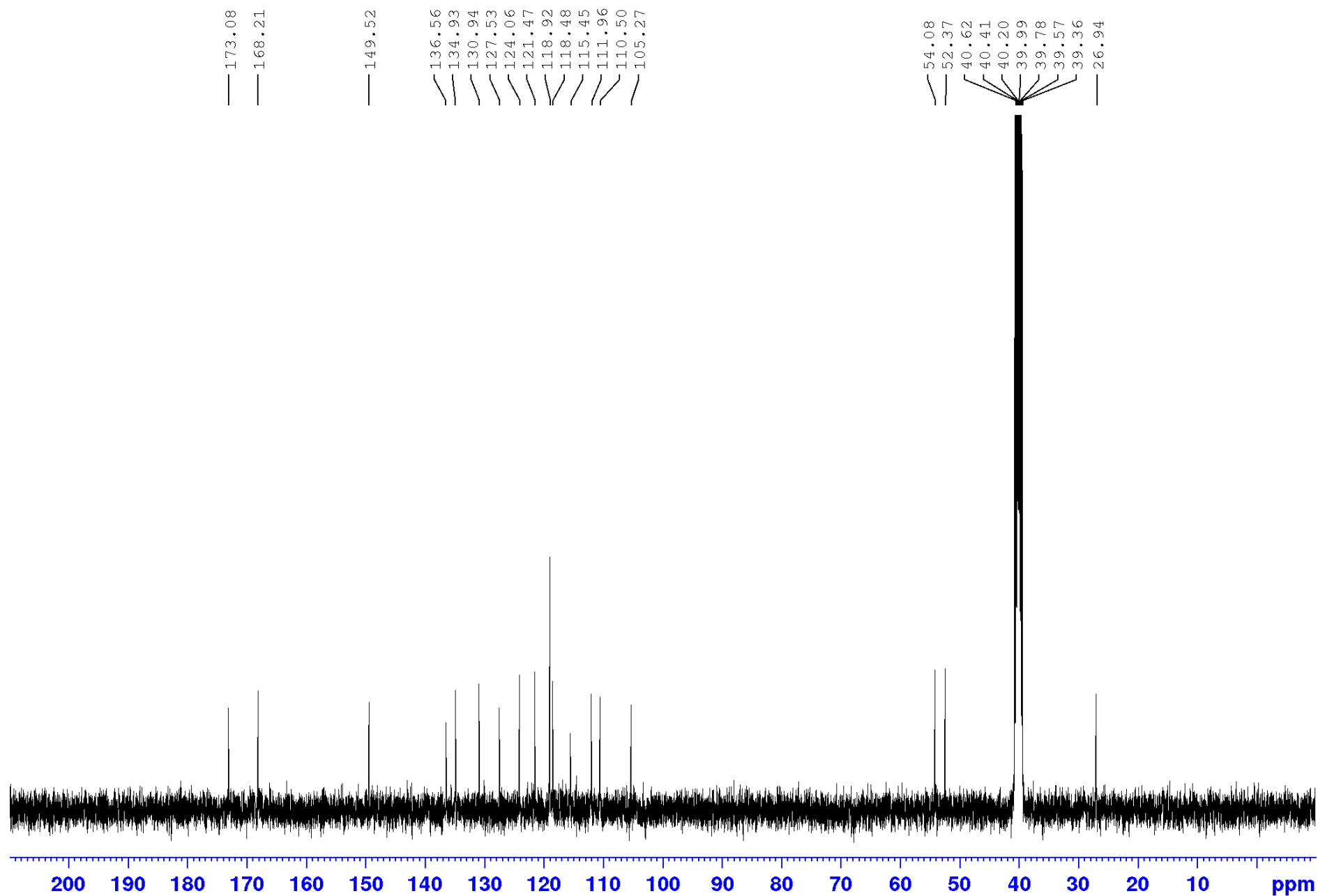
^{13}C NMR spectra of Methyl (2-amino-5-chlorobenzoyl)-*L*-tryptophanate (**2c**)



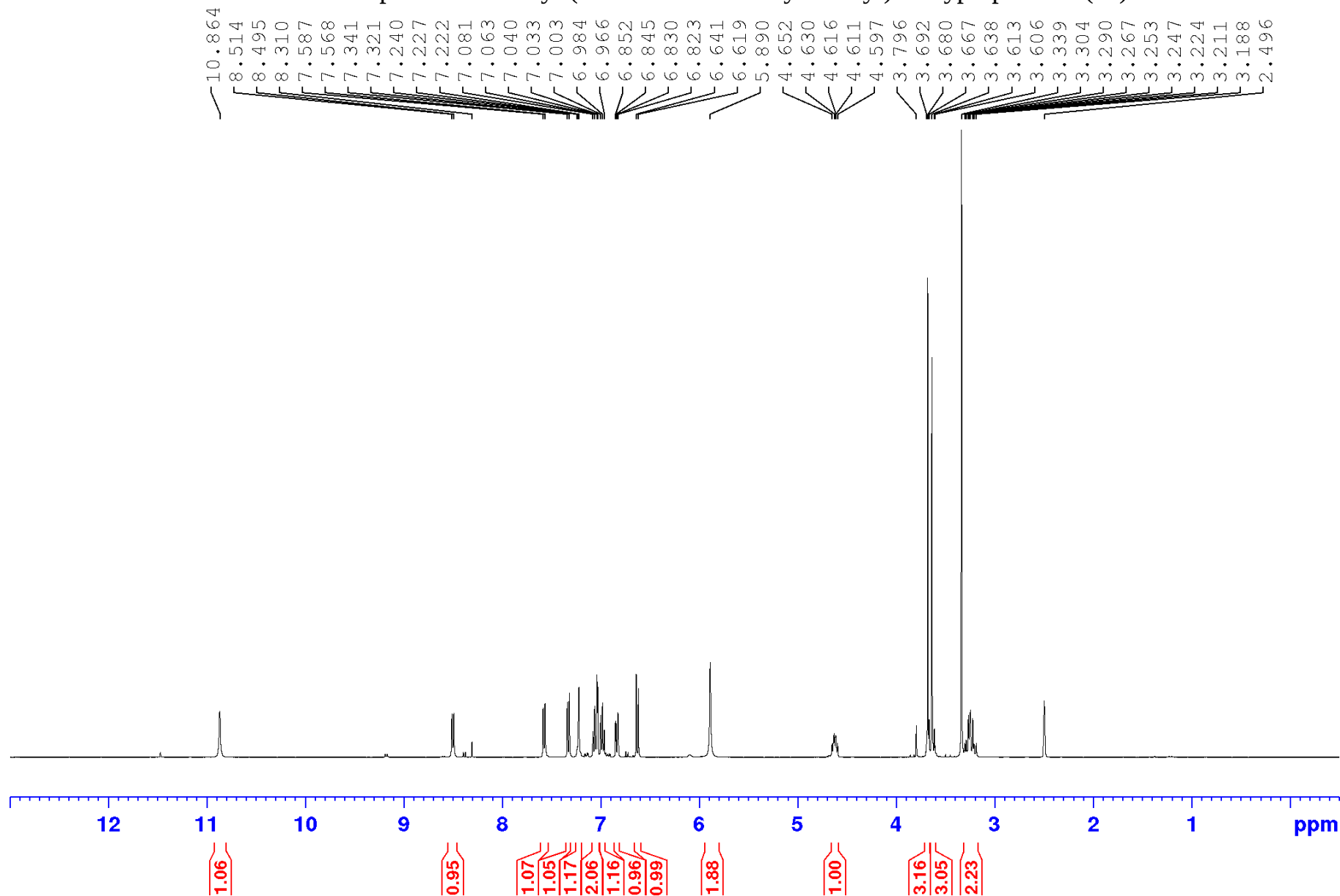
¹H NMR spectra of Methyl (2-amino-5-bromobenzoyl)-*L*-tryptophanate (**2d**)



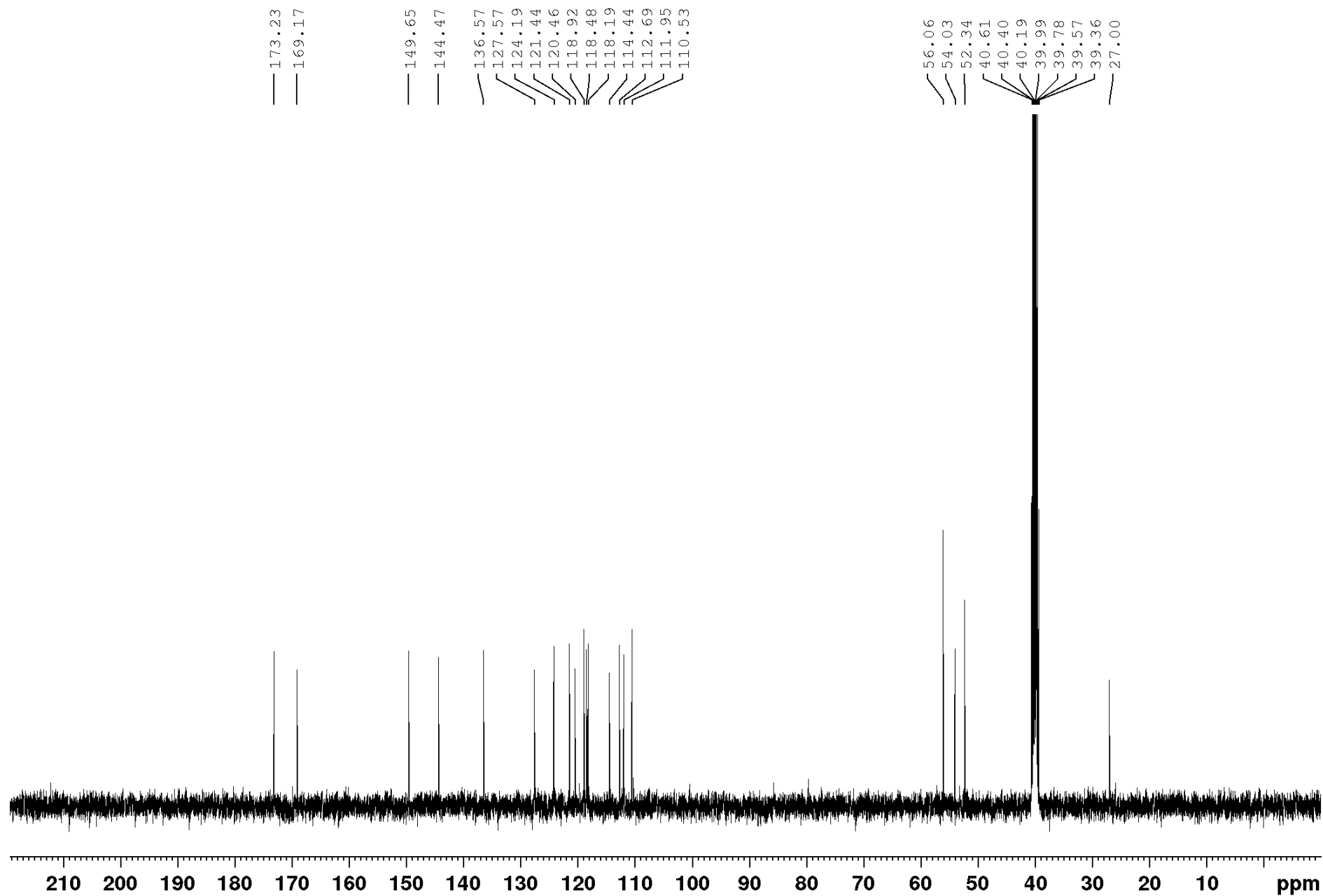
¹³C NMR spectra of Methyl (2-amino-5-bromobenzoyl)-L-tryptophanate (**2d**)



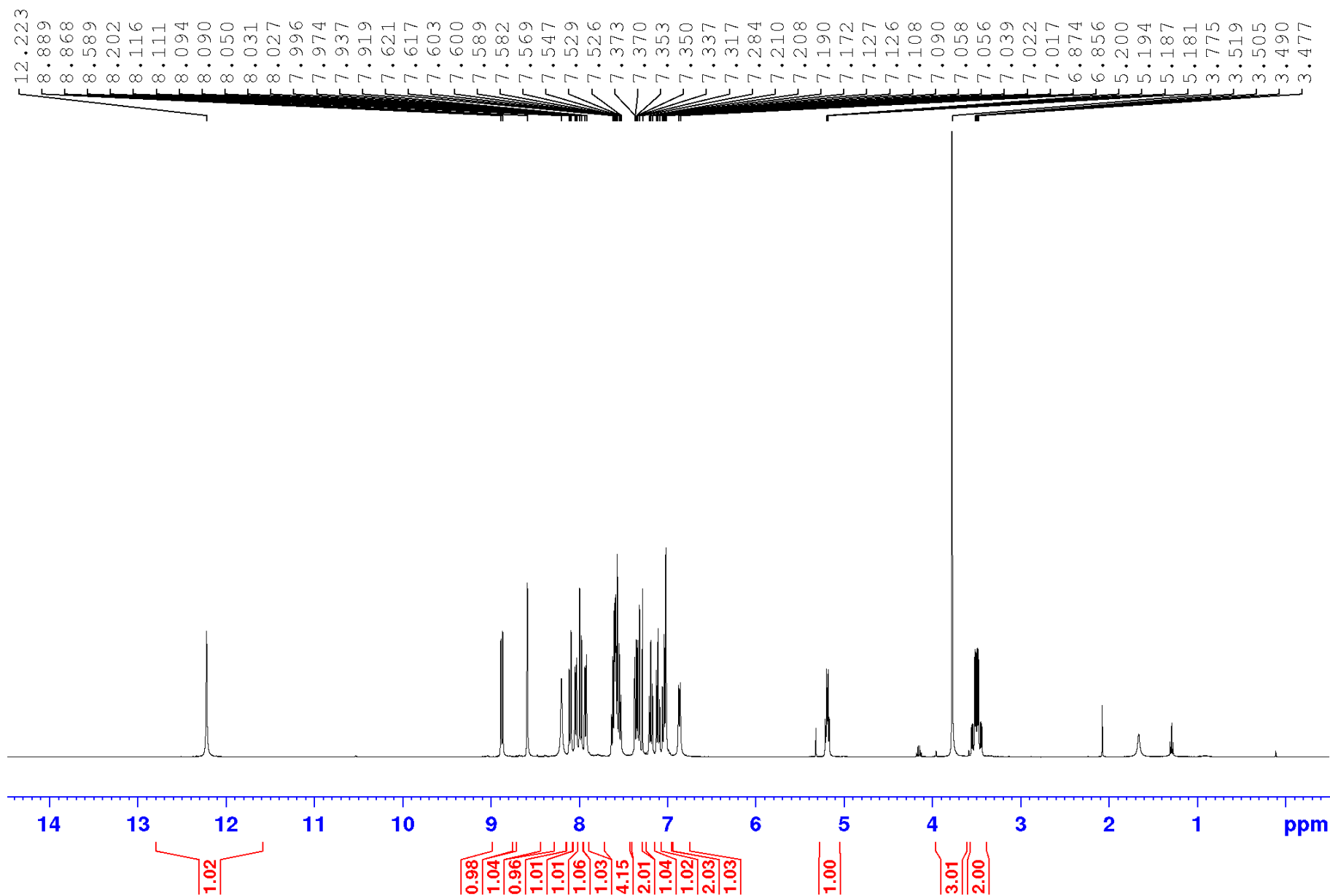
¹H NMR spectra of Methyl (2-amino-5-methoxybenzoyl)-L-tryptophanate (**2e**)



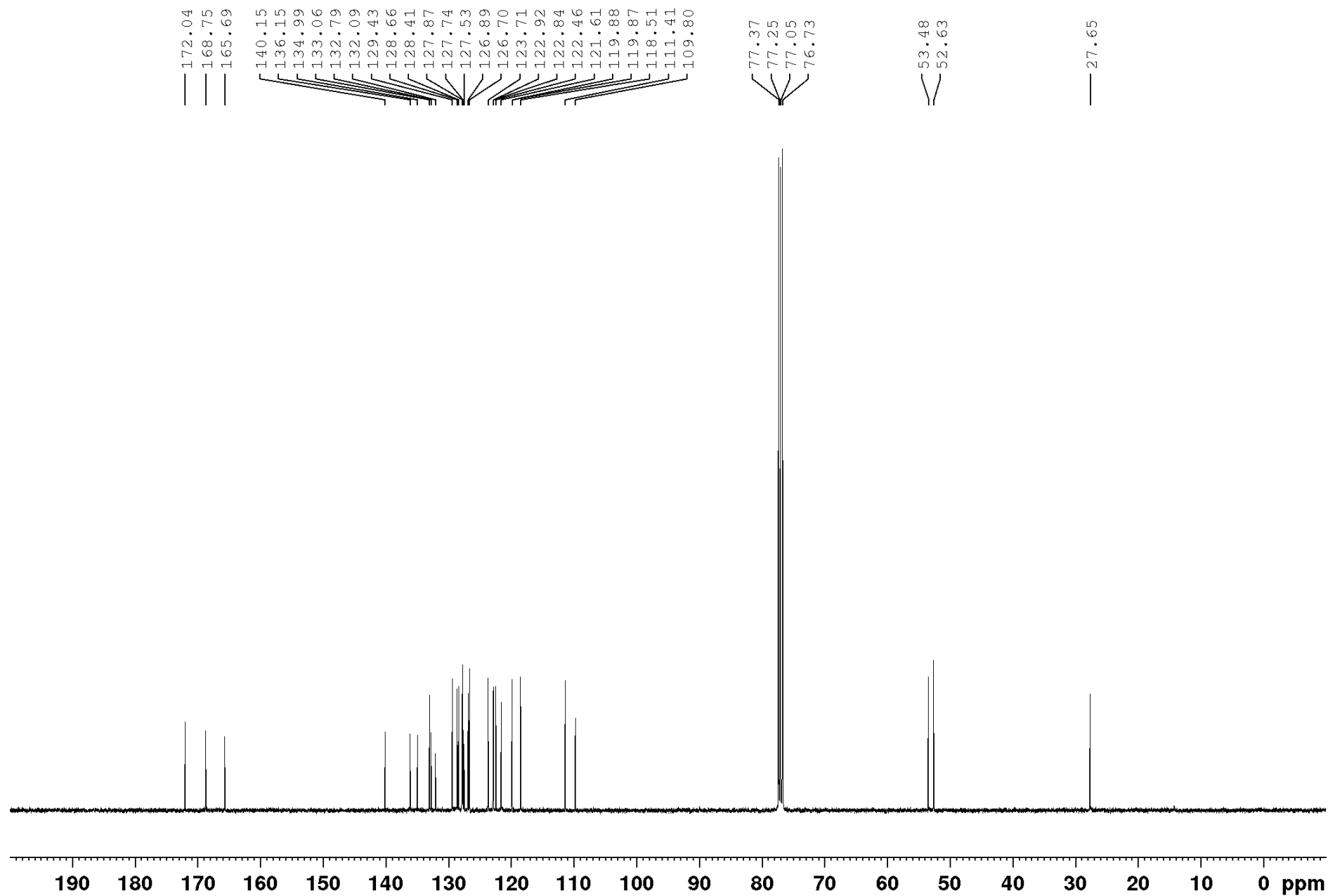
¹³C NMR spectra of Methyl (2-amino-5-methoxybenzoyl)-*L*-tryptophanate (**2e**)



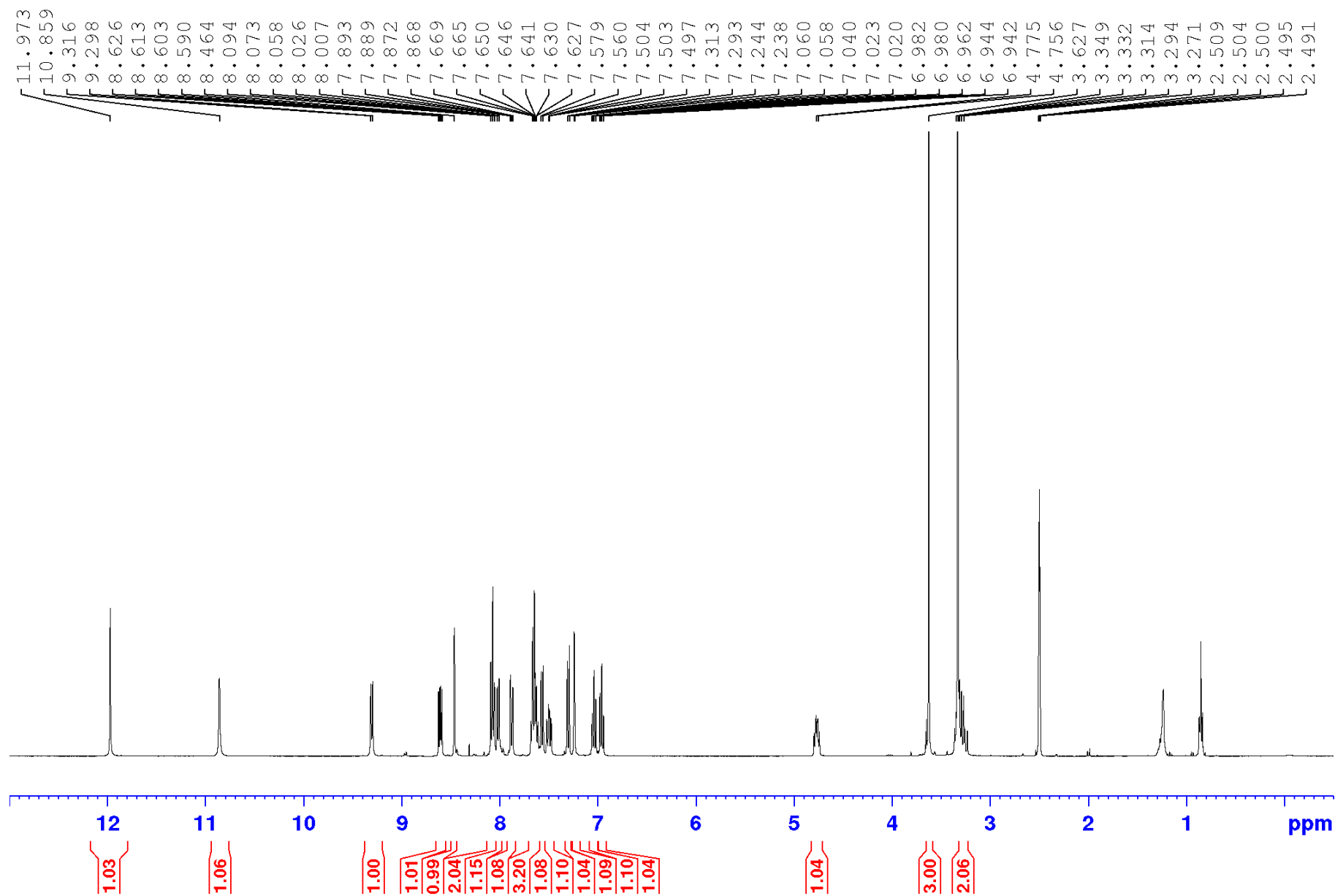
¹H NMR spectra of Methyl (2-(2-naphthamido)benzoyl)-L-tryptophanate (**3a**)



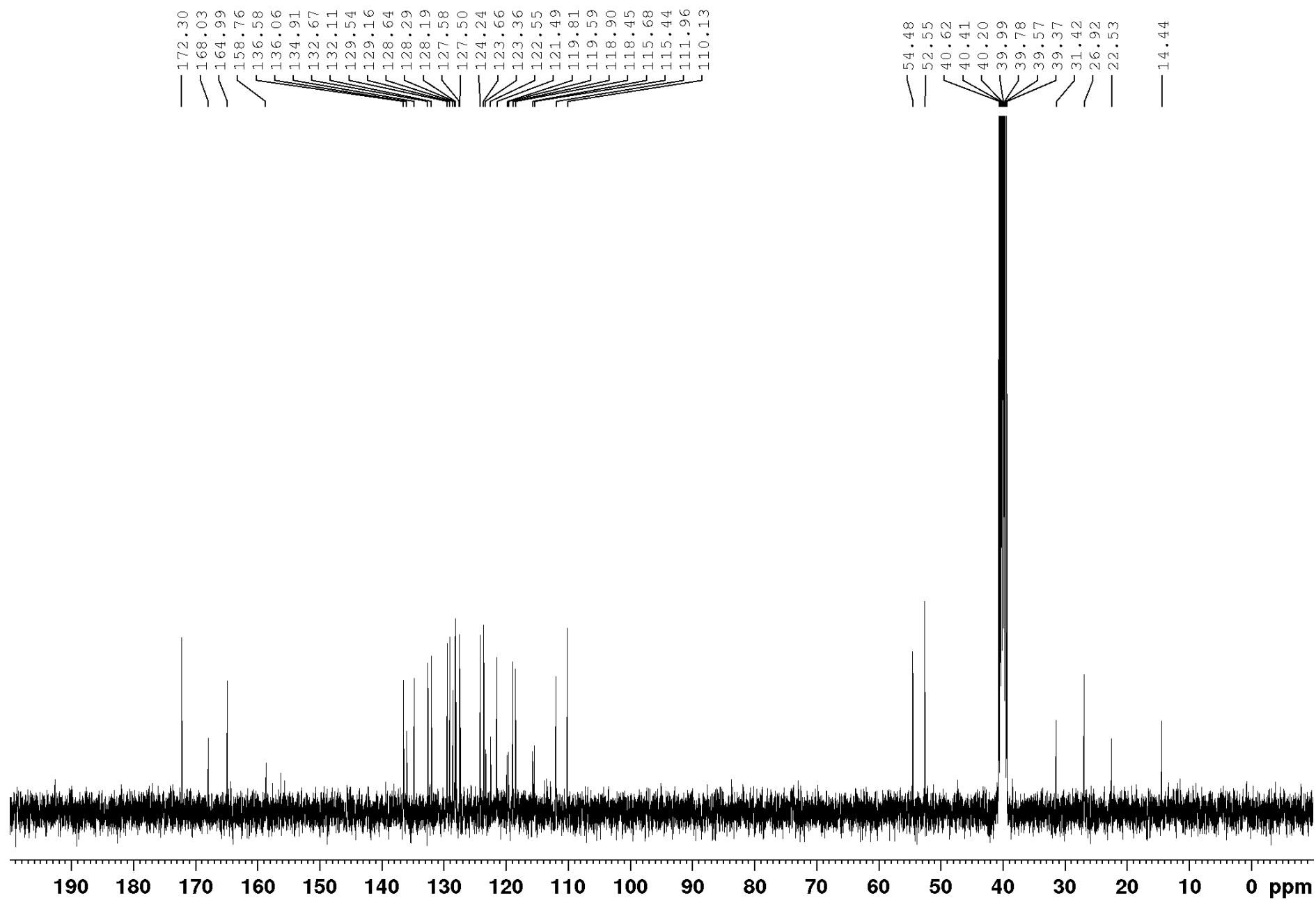
^{13}C NMR spectra of Methyl (2-(2-naphthamido)benzoyl)-*L*-tryptophanate (**3a**)



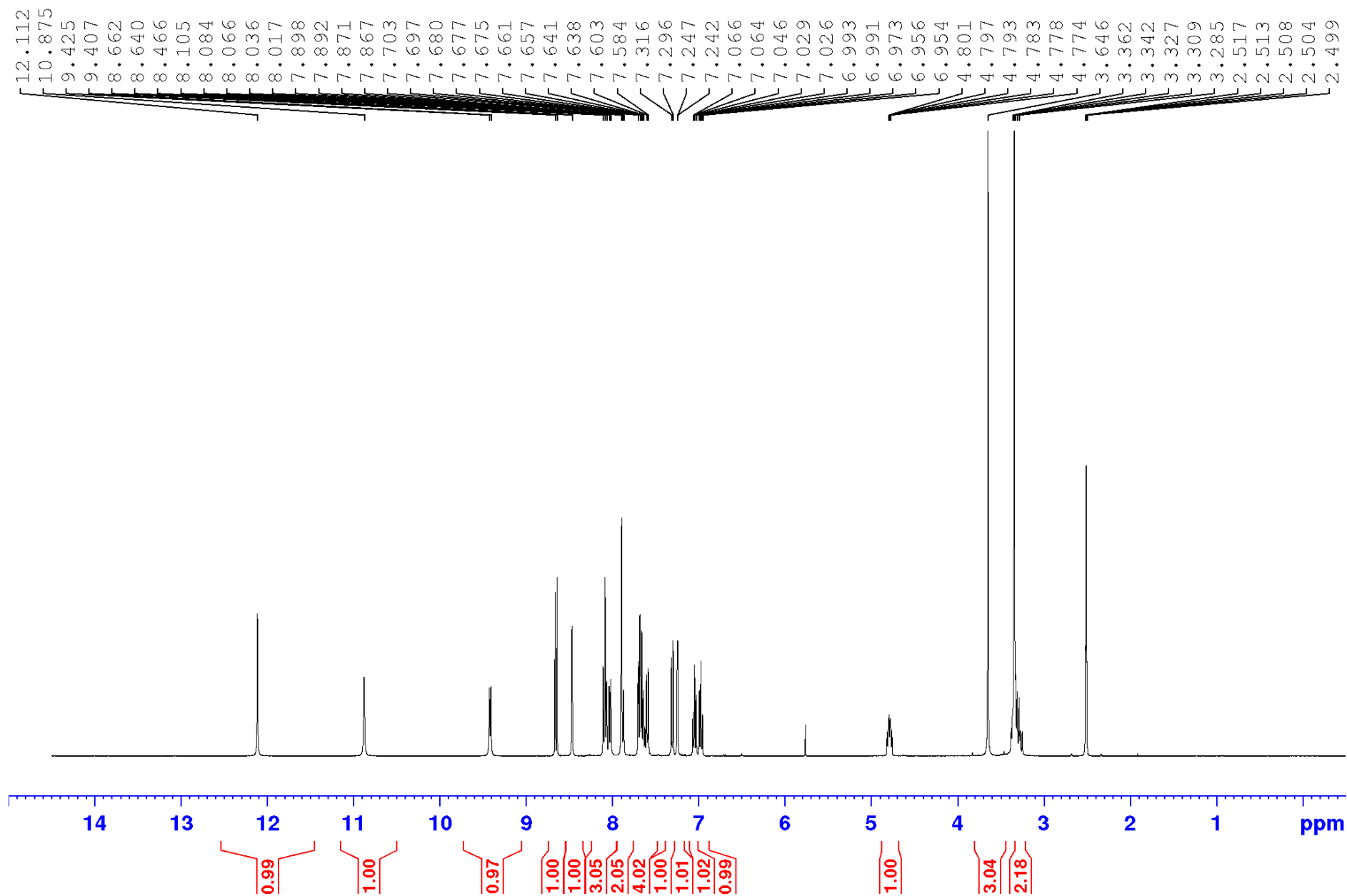
¹H NMR spectra of Methyl (2-(2-naphthamido)-5-fluorobenzoyl)-L-tryptophanate (**3b**)



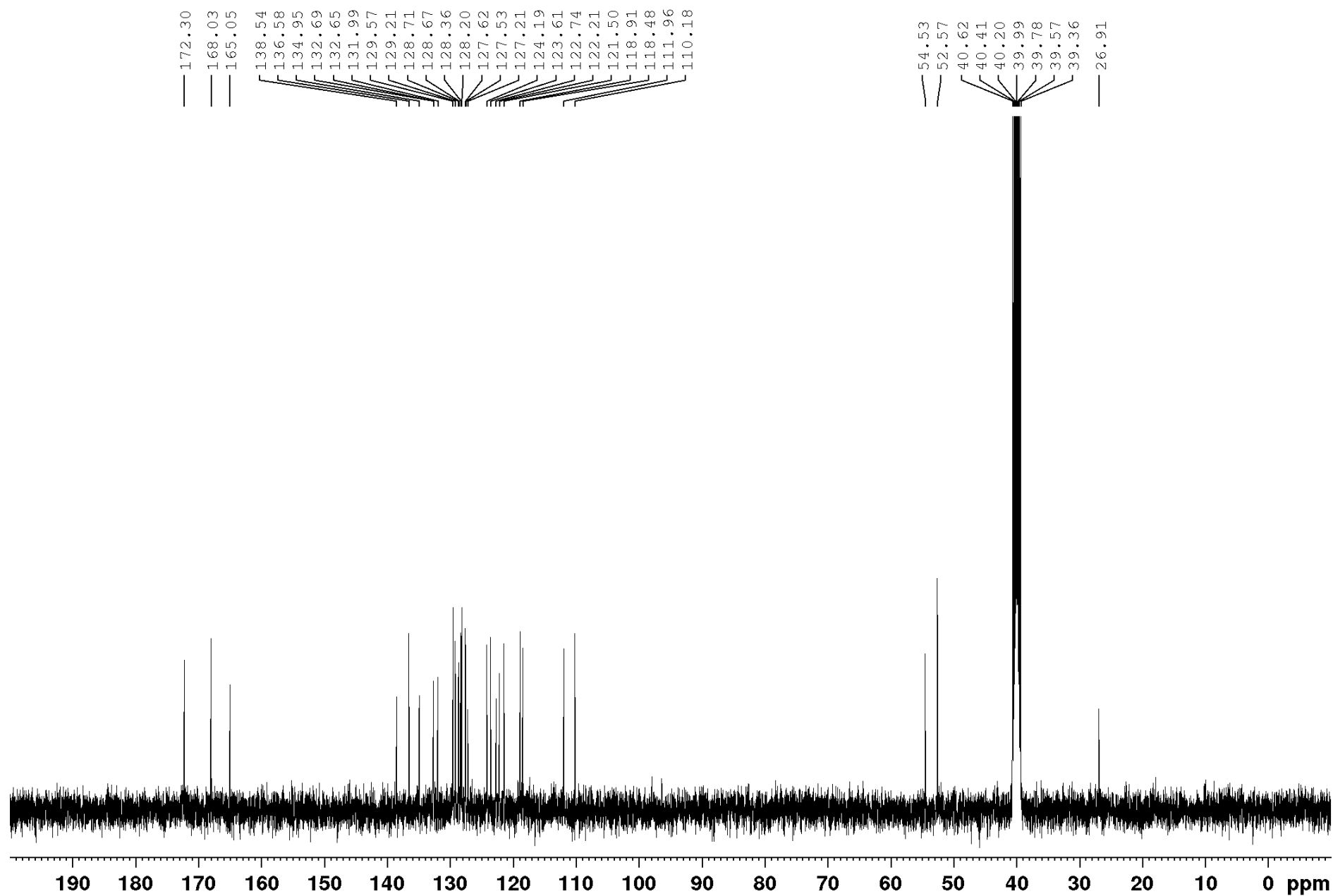
¹³C NMR spectra of Methyl (2-(2-naphthamido)-5-fluorobenzoyl)-*L*-tryptophanate (**3b**)



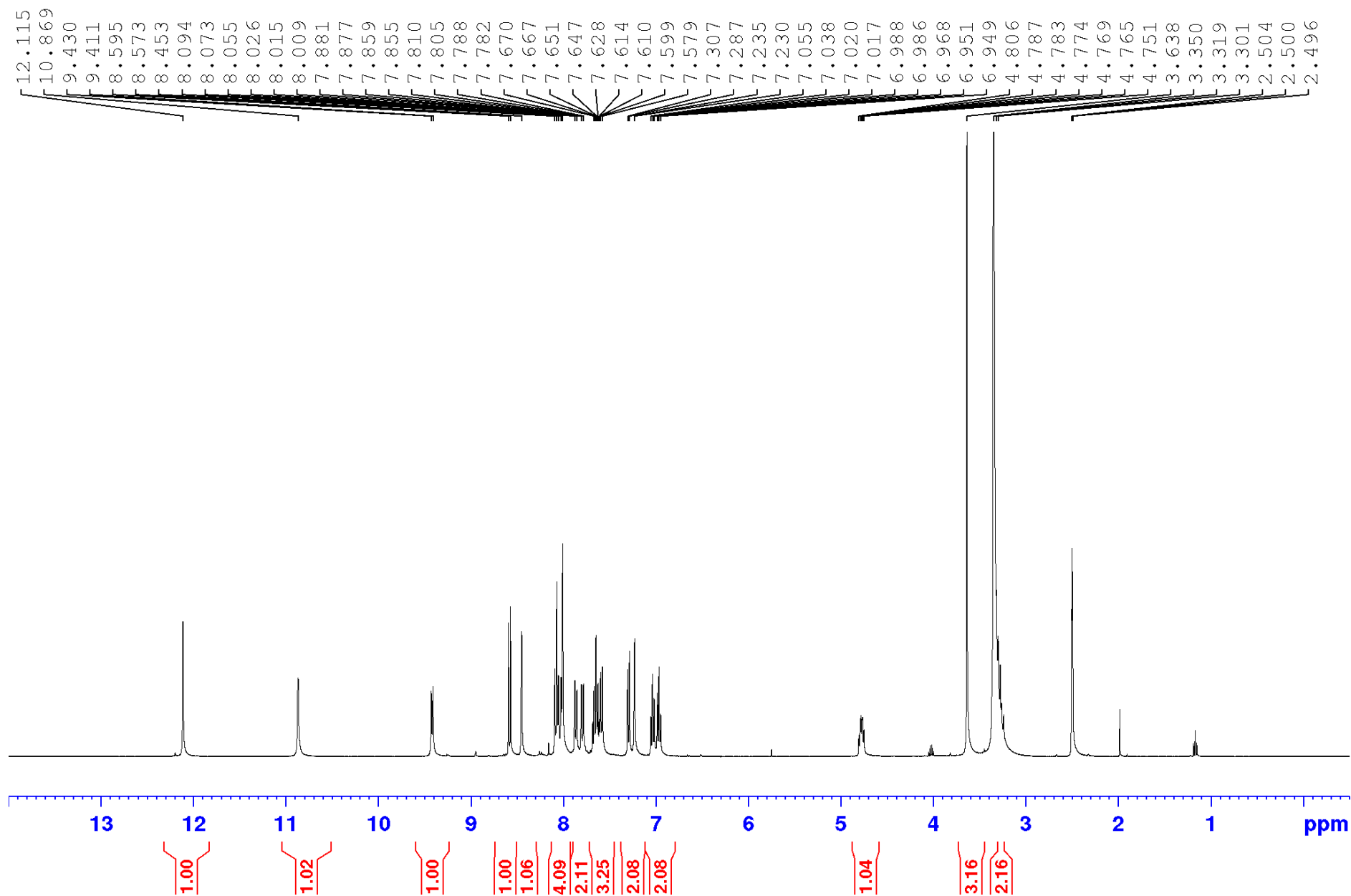
¹H NMR spectra of Methyl (2-(2-naphthamido)-5-chlorobenzoyl)-L-tryptophanate (**3c**)



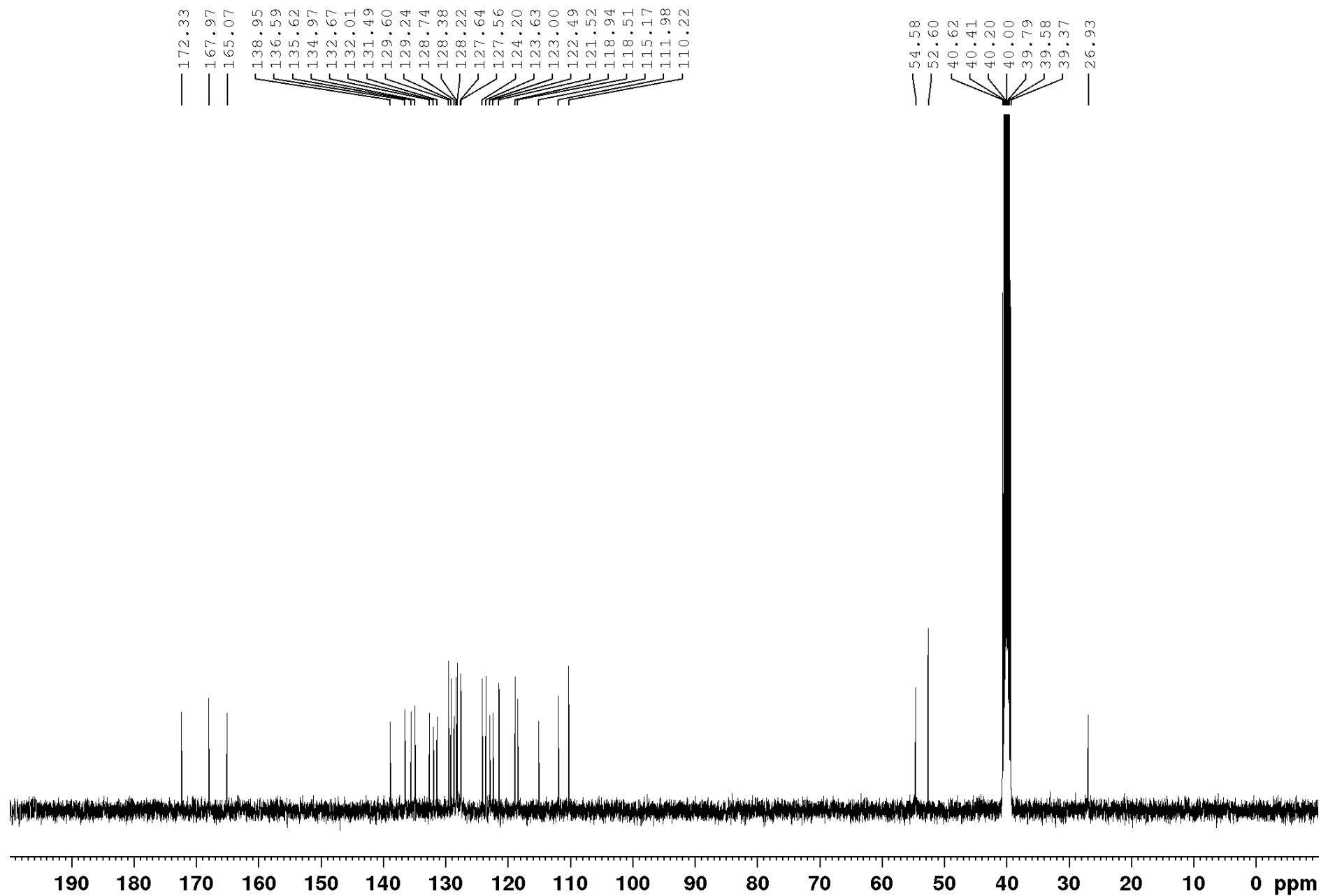
^{13}C NMR spectra of Methyl (2-(2-naphthamido)-5-chlorobenzoyl)-*L*-tryptophanate (**3c**)



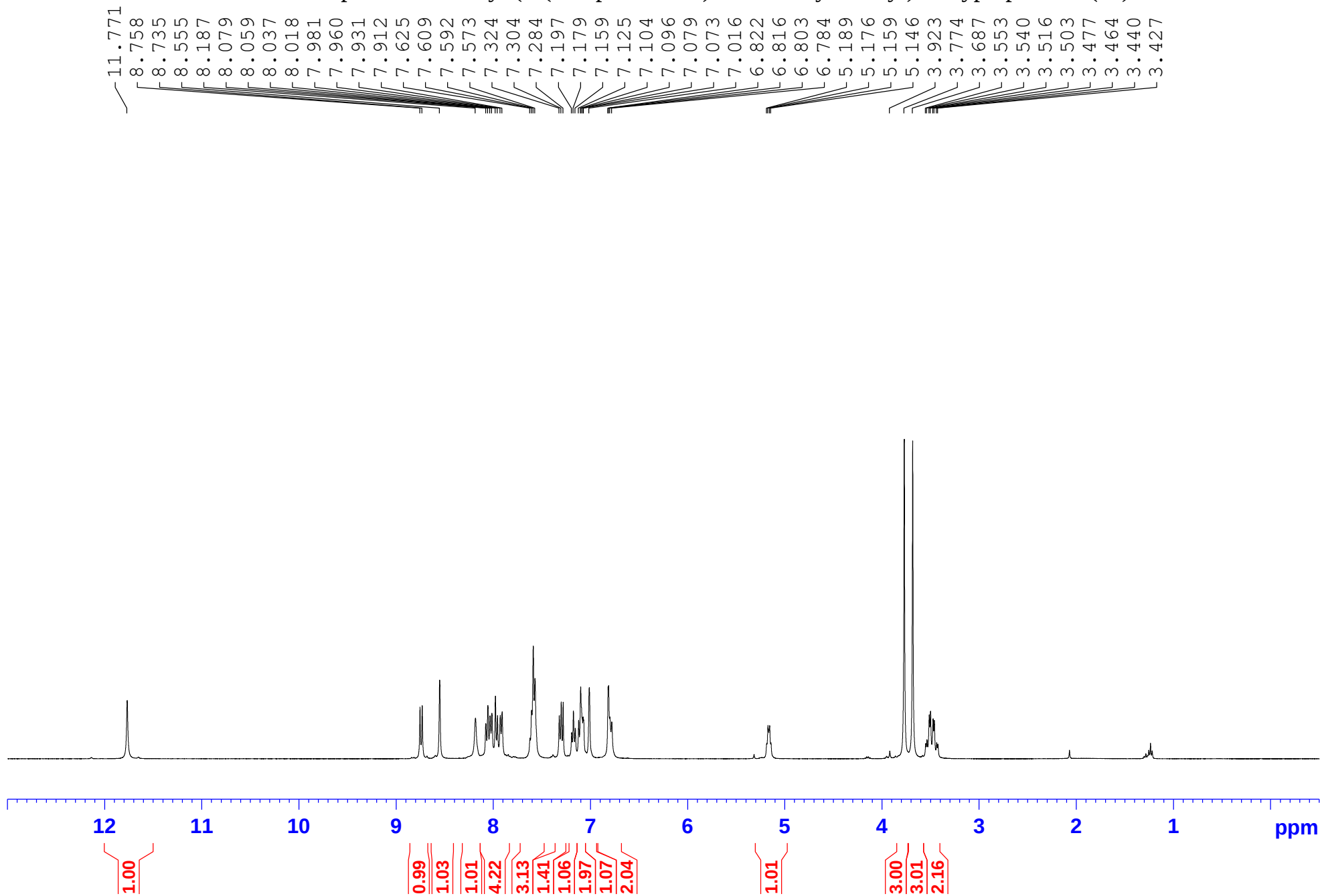
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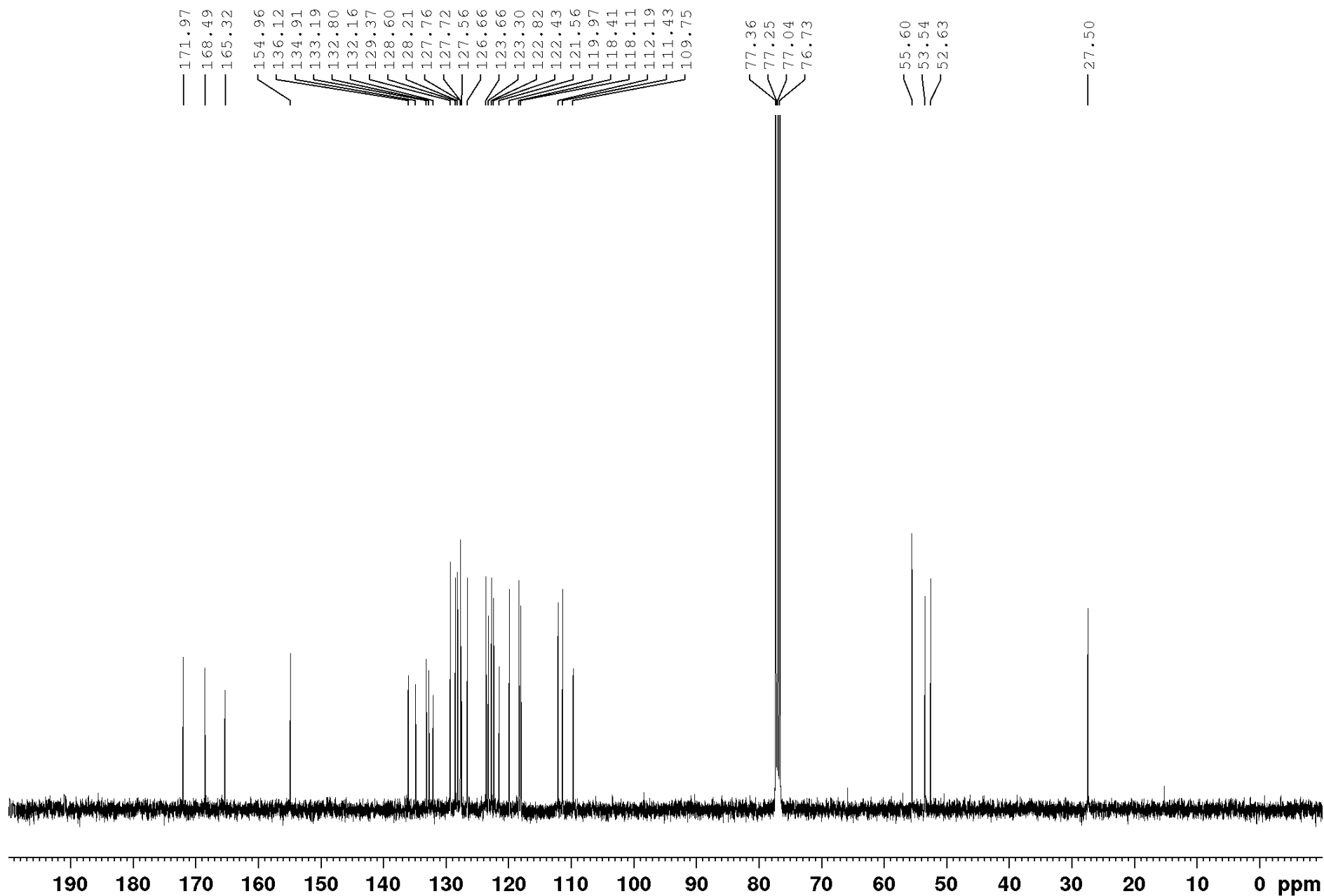
^{13}C NMR spectra of Methyl (2-(2-naphthamido)-5-bromobenzoyl)-*L*-tryptophanate (**3d**)



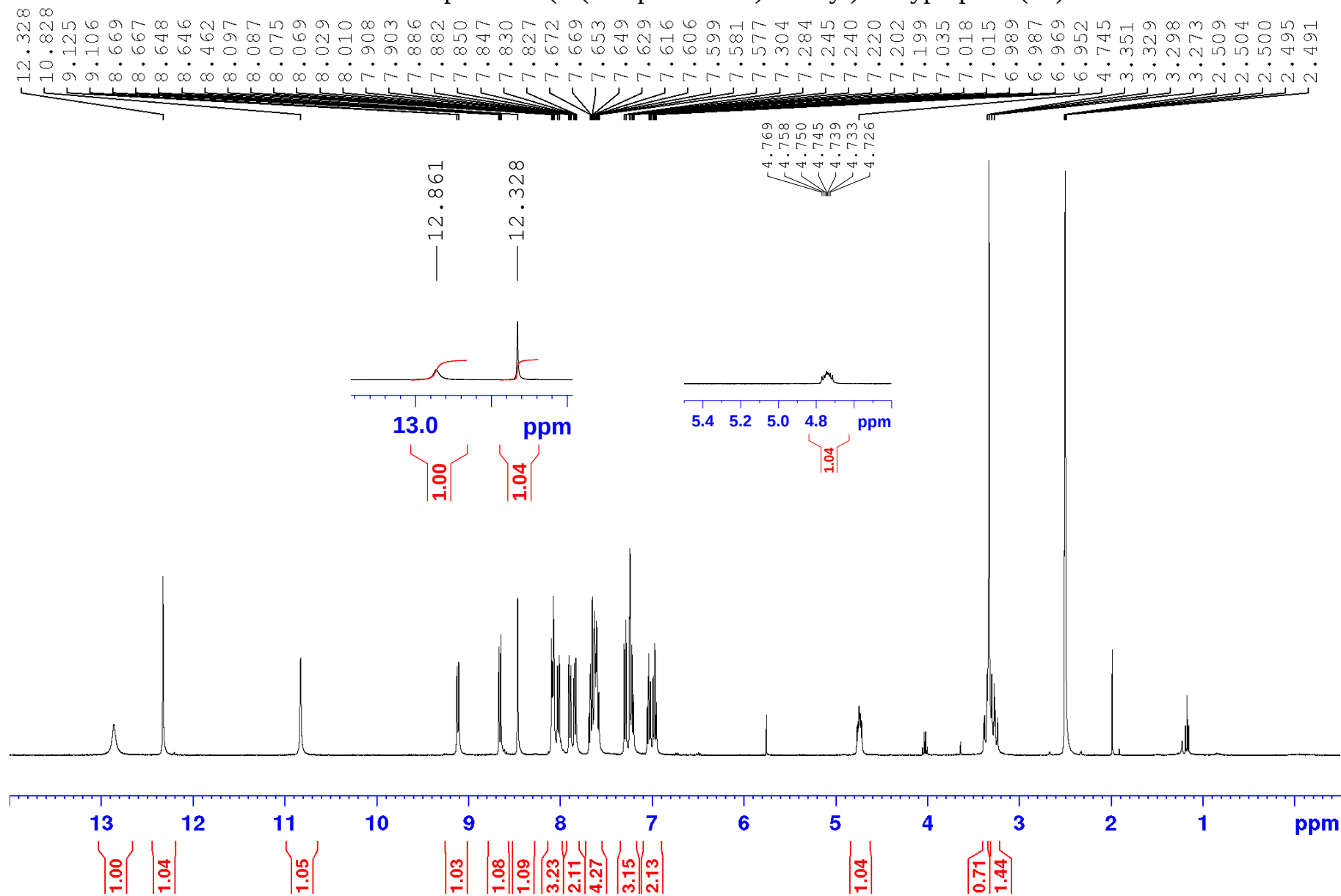
¹H NMR spectra of Methyl (2-(2-naphthamido)-5-methoxybenzoyl)-*L*-tryptophanate (**3e**)



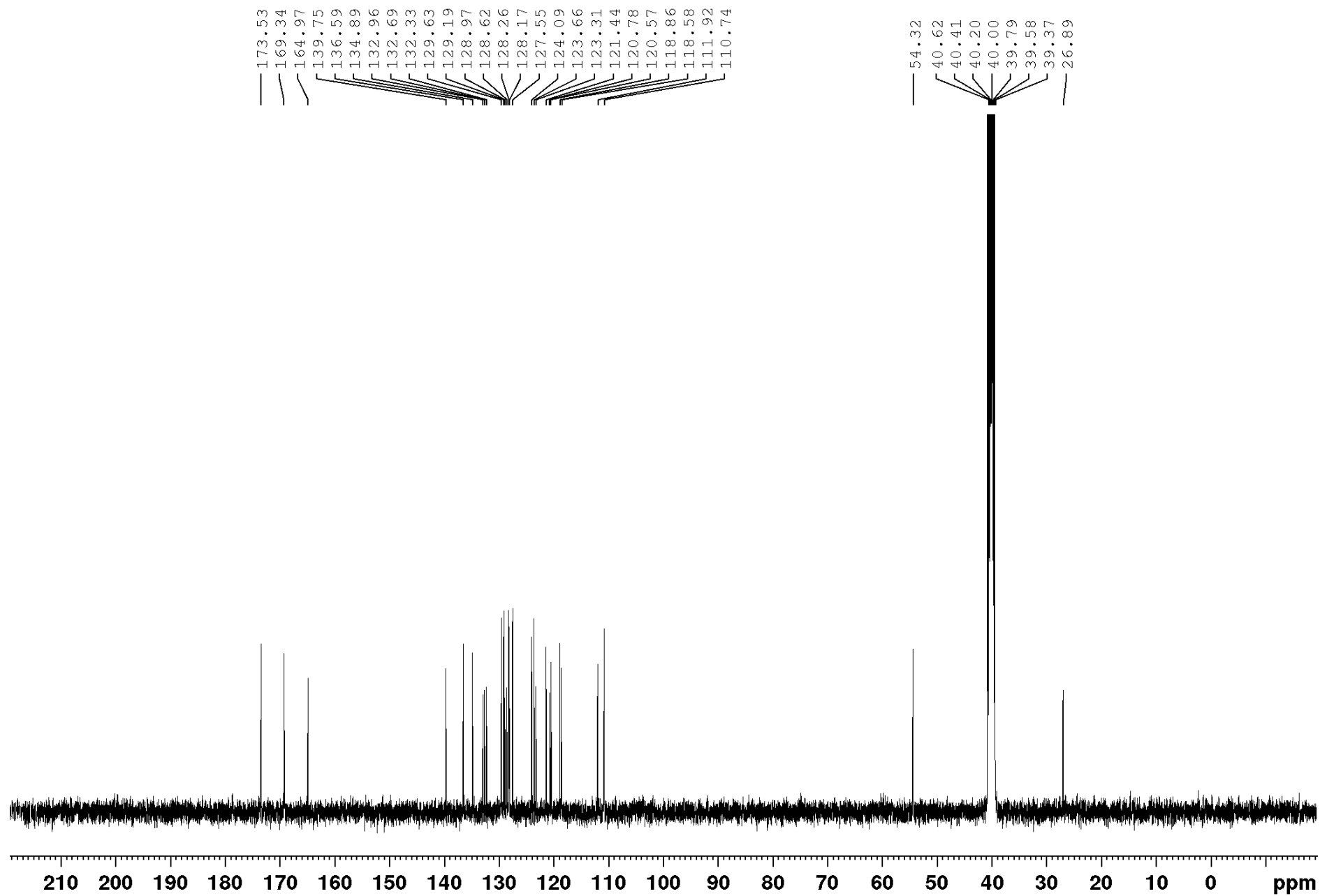
¹³C NMR spectra of Methyl (2-(2-naphthamido)-5-methoxybenzoyl)-*L*-tryptophanate (**3e**)



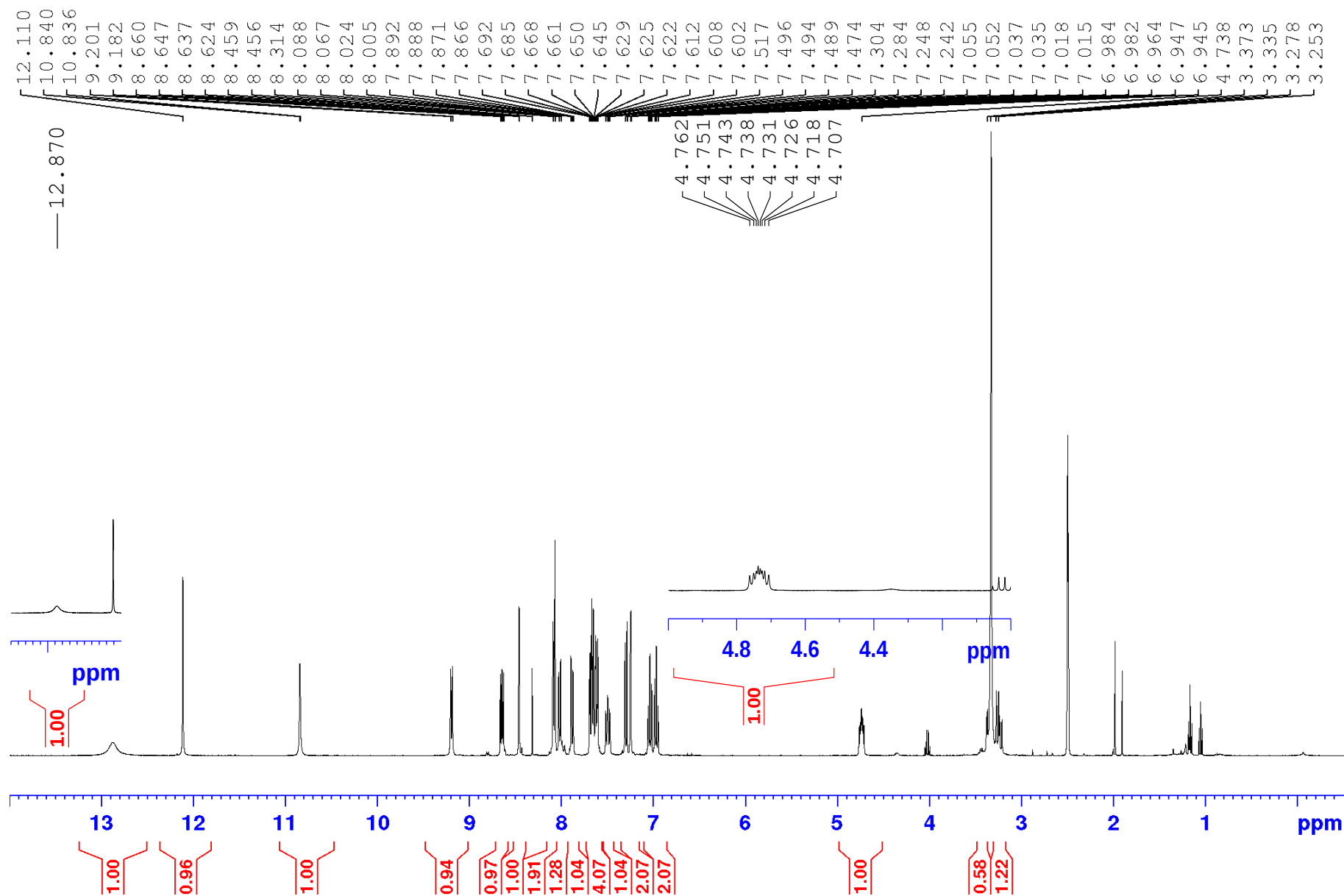
¹H NMR spectra of (2-(2-naphthamido)benzoyl)-L-tryptophan (**4a**)



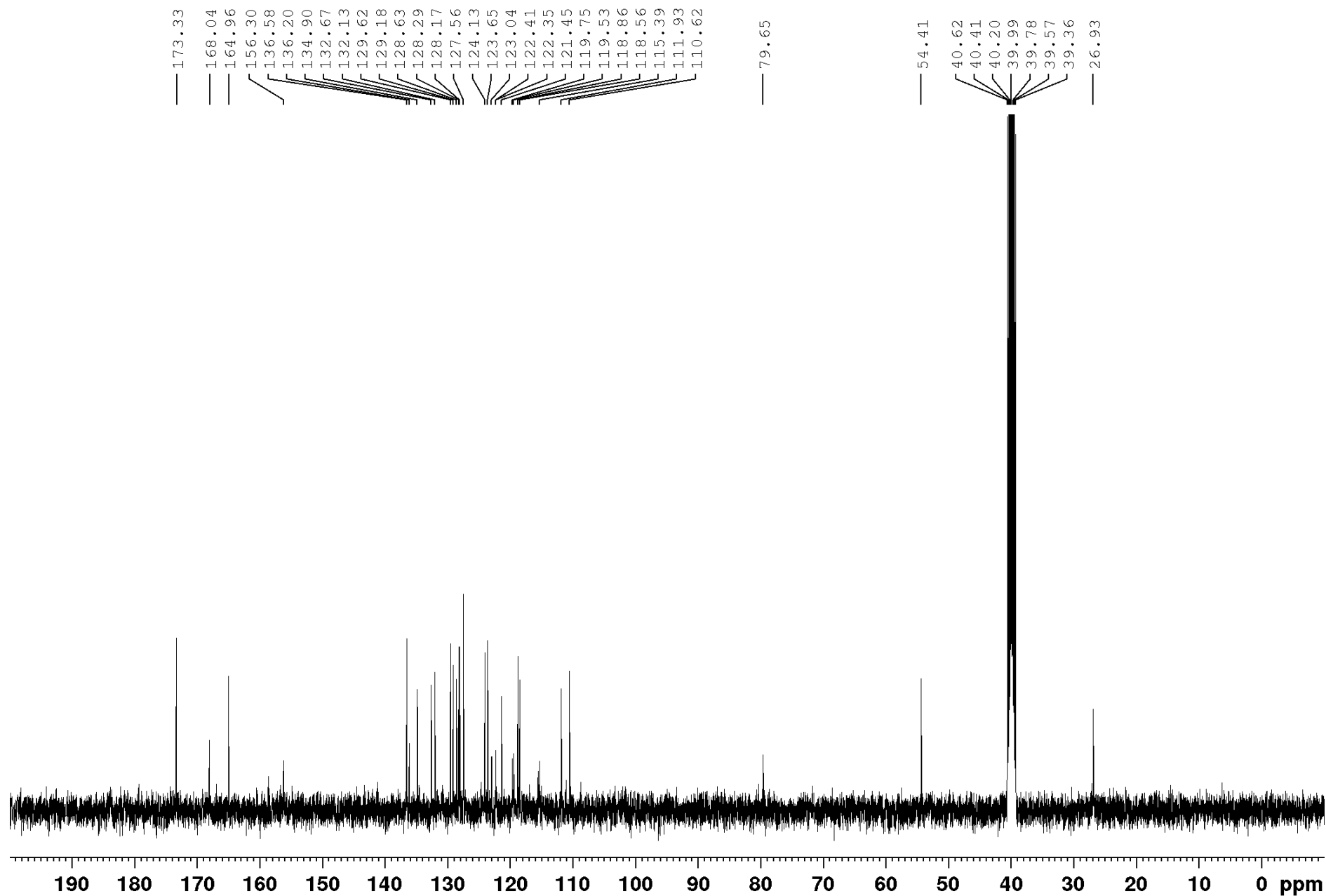
^{13}C NMR spectra of (2-(2-naphthamido)benzoyl)-*L*-tryptophan (**4a**)



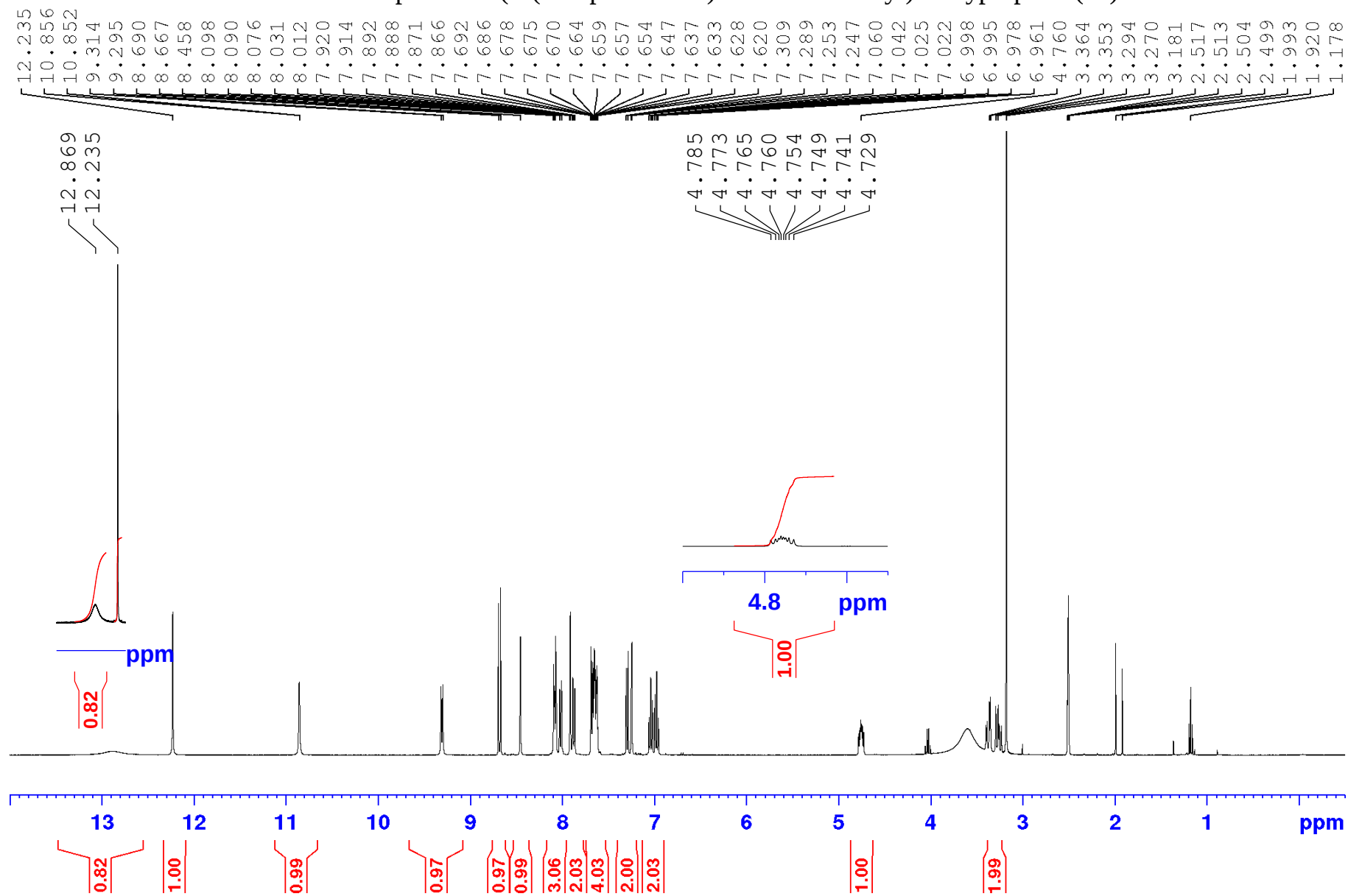
¹H NMR spectra of (2-(2-naphthamido)-5-fluorobenzoyl)-L-tryptophan (**4b**)



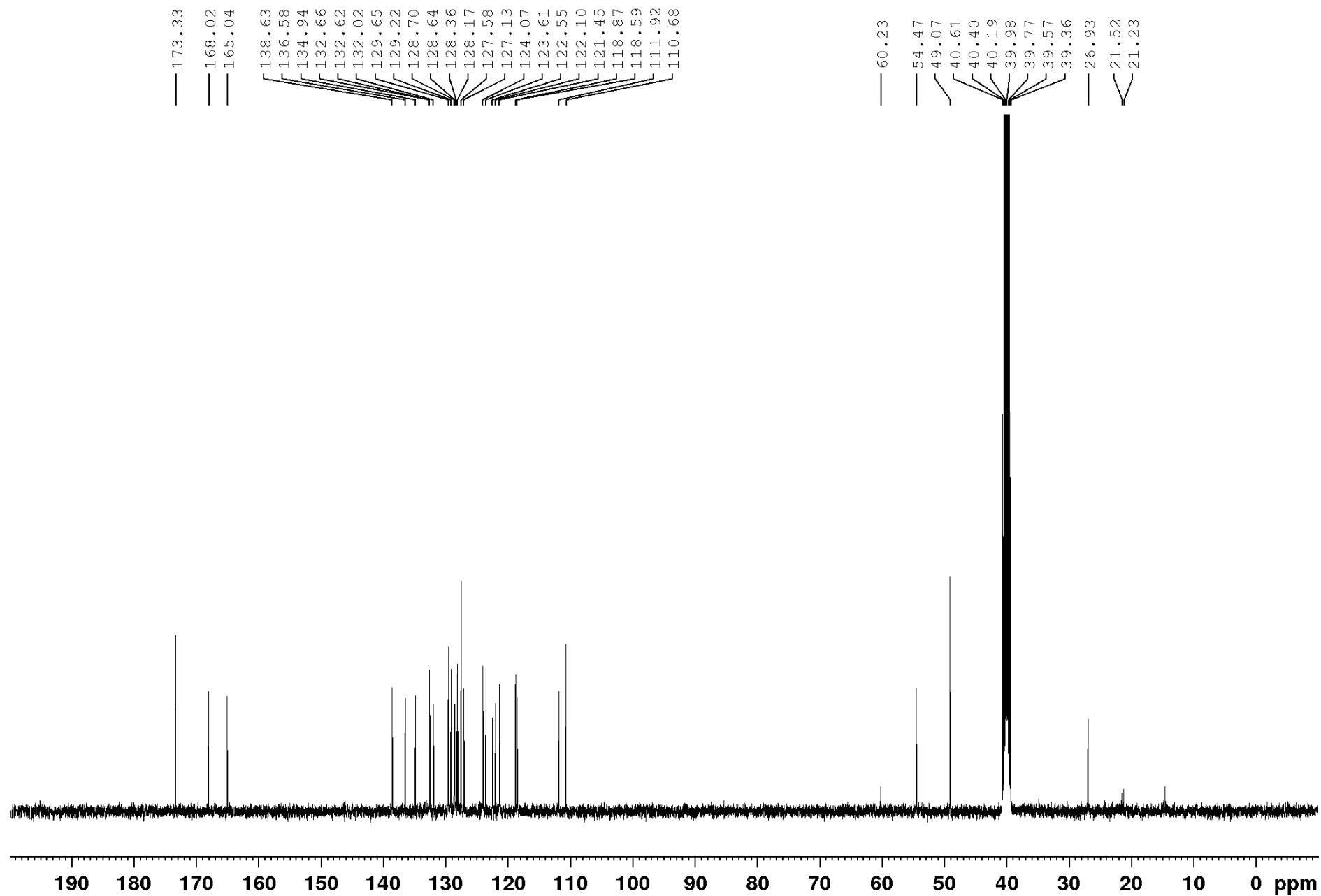
^{13}C NMR spectra of (2-(2-naphthamido)-5-fluorobenzoyl)-L-tryptophan (**4b**)



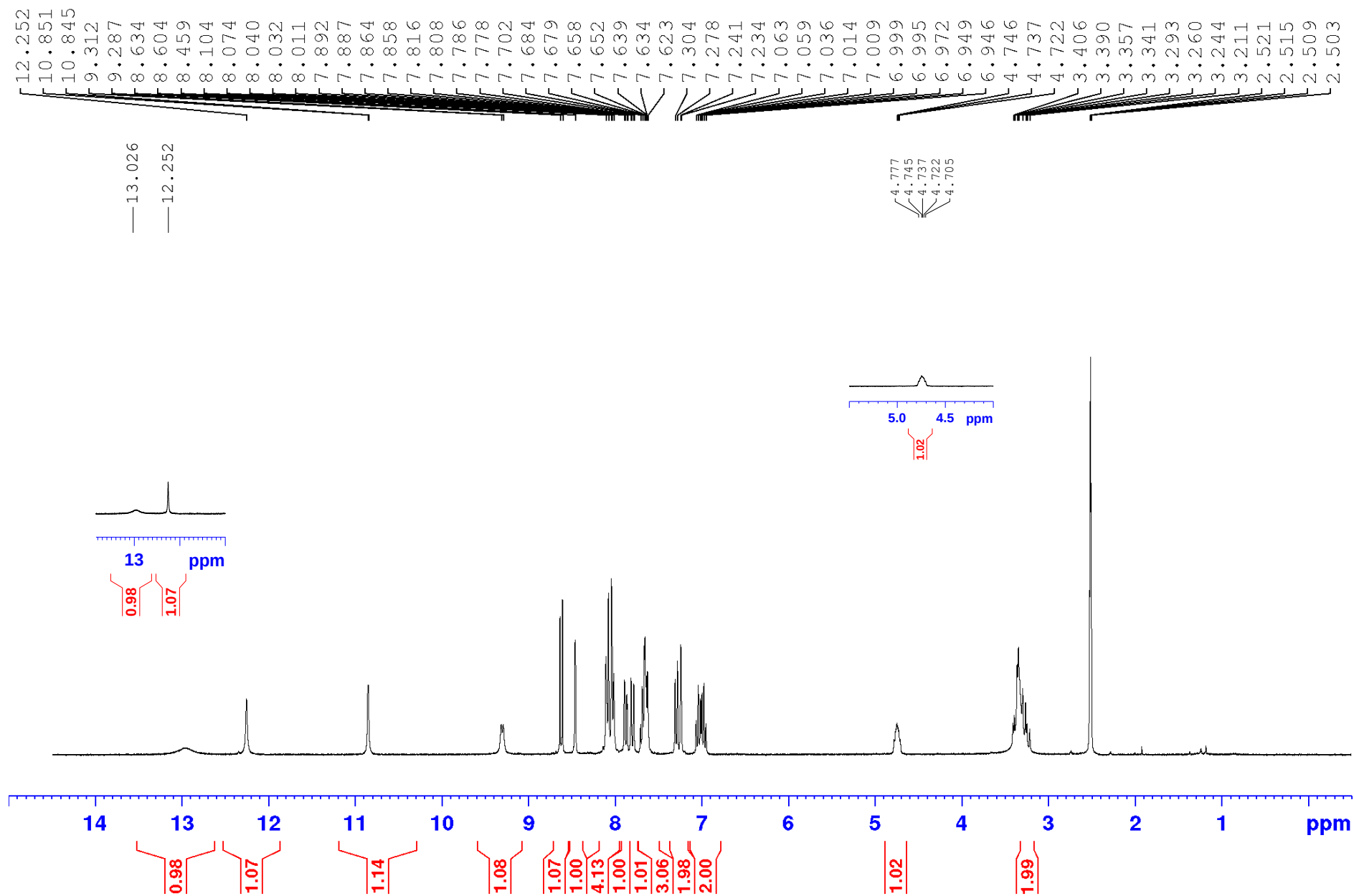
¹H NMR spectra of (2-(2-naphthamido)-5-chlorobenzoyl)-L-tryptophan (**4c**)



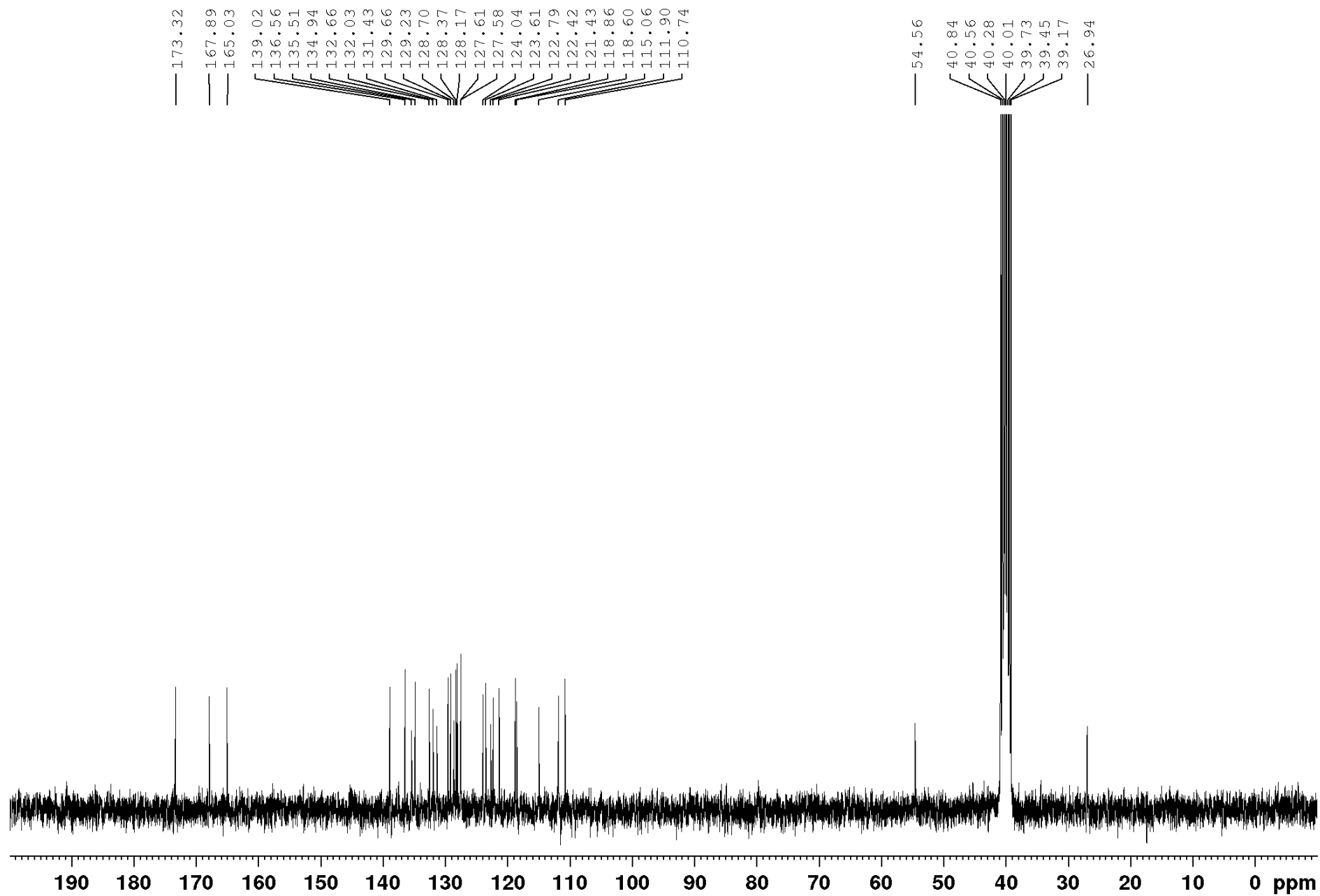
^{13}C NMR spectra of (2-(2-naphthamido)-5-chlorobenzoyl)-*L*-tryptophan (**4c**)



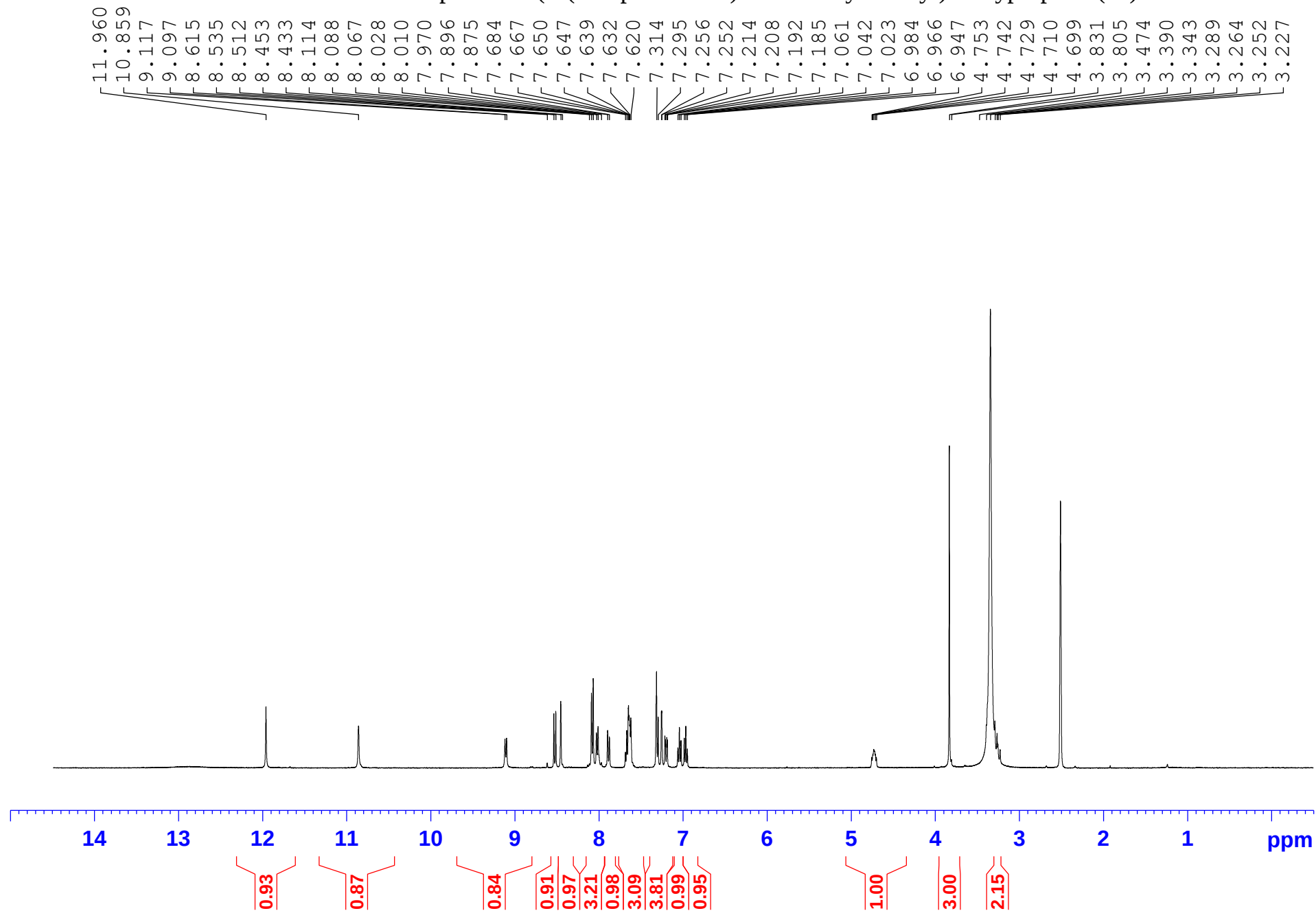
¹H NMR spectra of (2-(2-naphthamido)-5-bromobenzoyl)-L-tryptophan (**4d**)



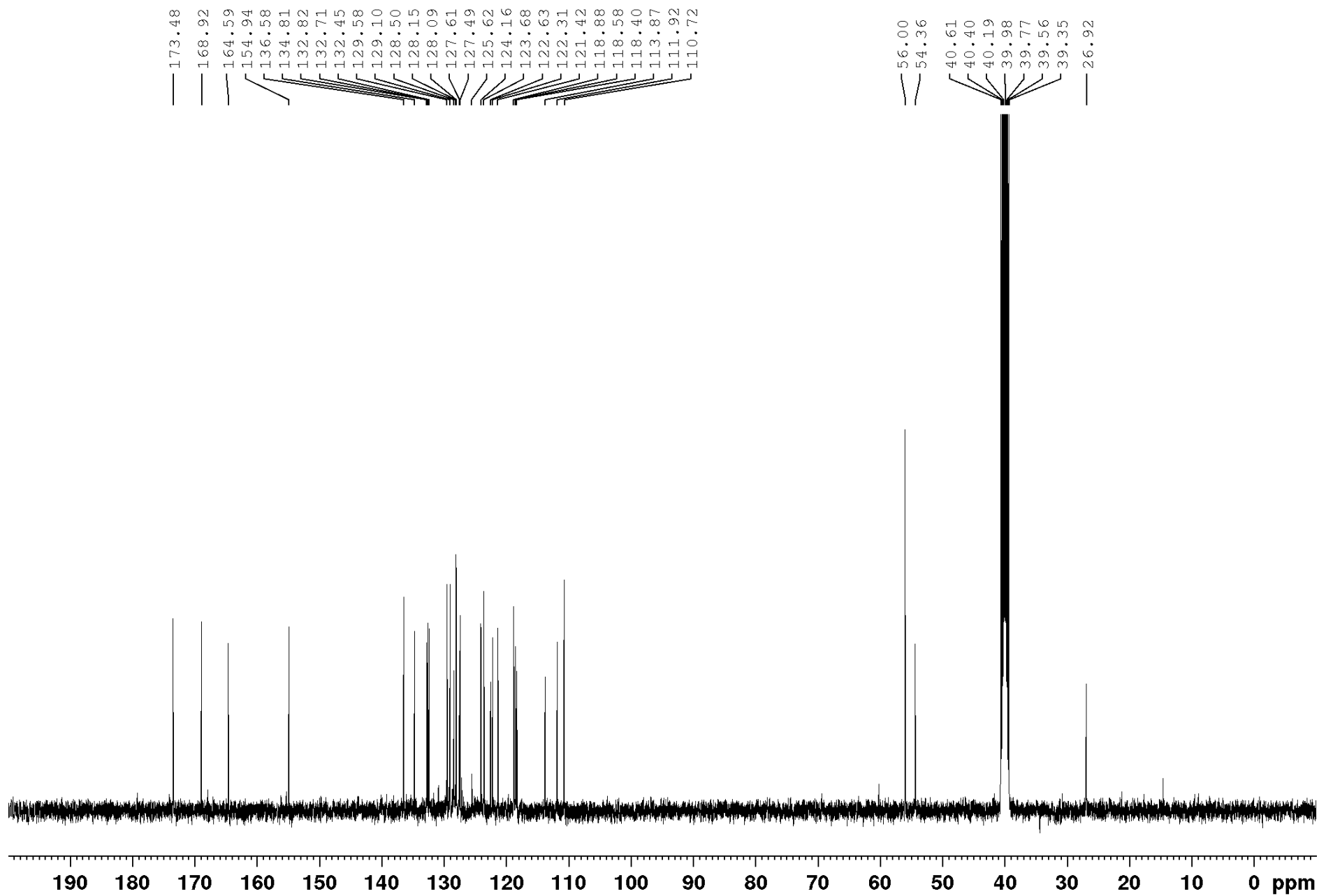
^{13}C NMR spectra of (2-(2-naphthamido)-5-bromobenzoyl)-*L*-tryptophan (**4d**)



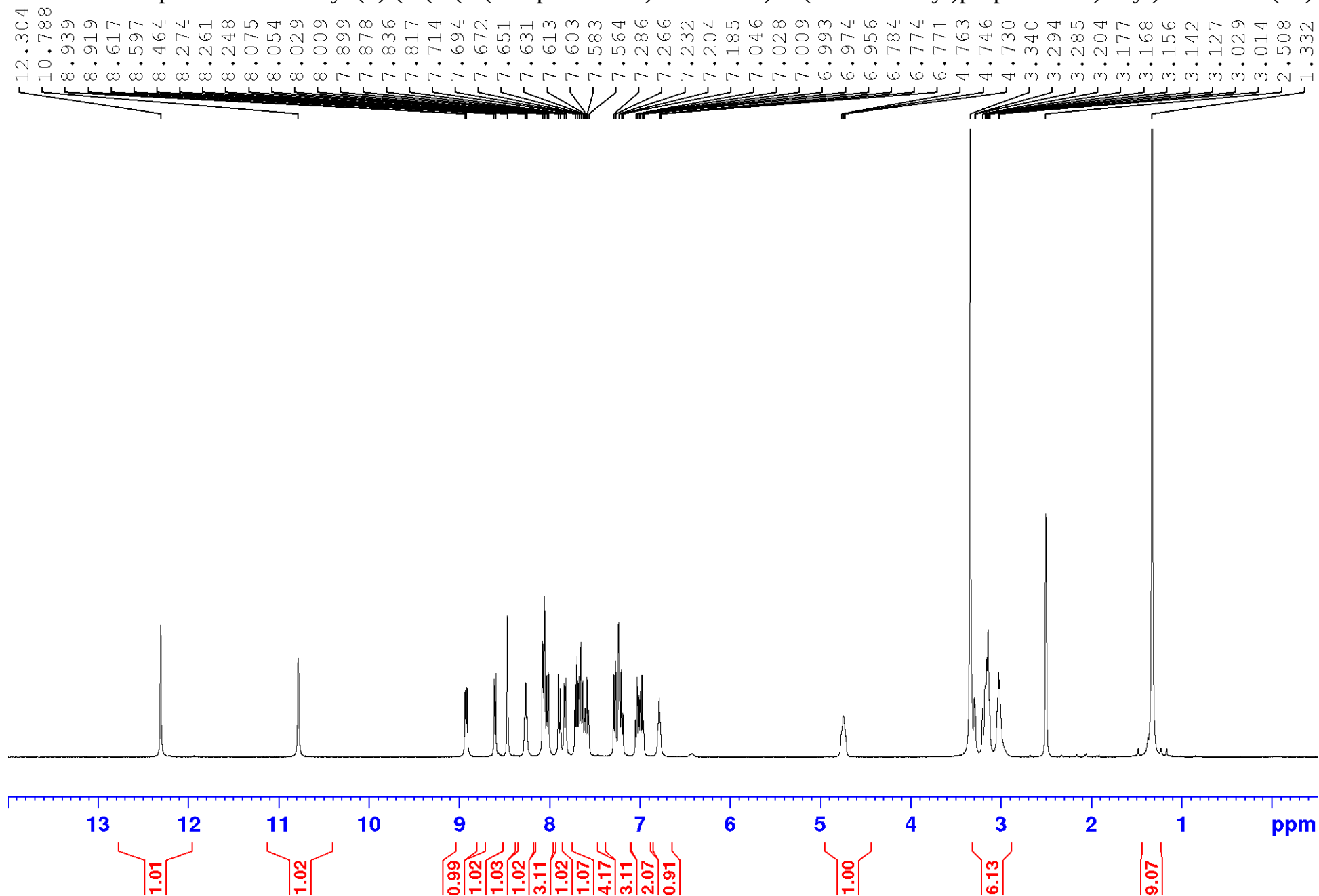
¹H NMR spectra of (2-(2-naphthamido)-5-methoxybenzoyl)-*L*-tryptophan (**4e**)



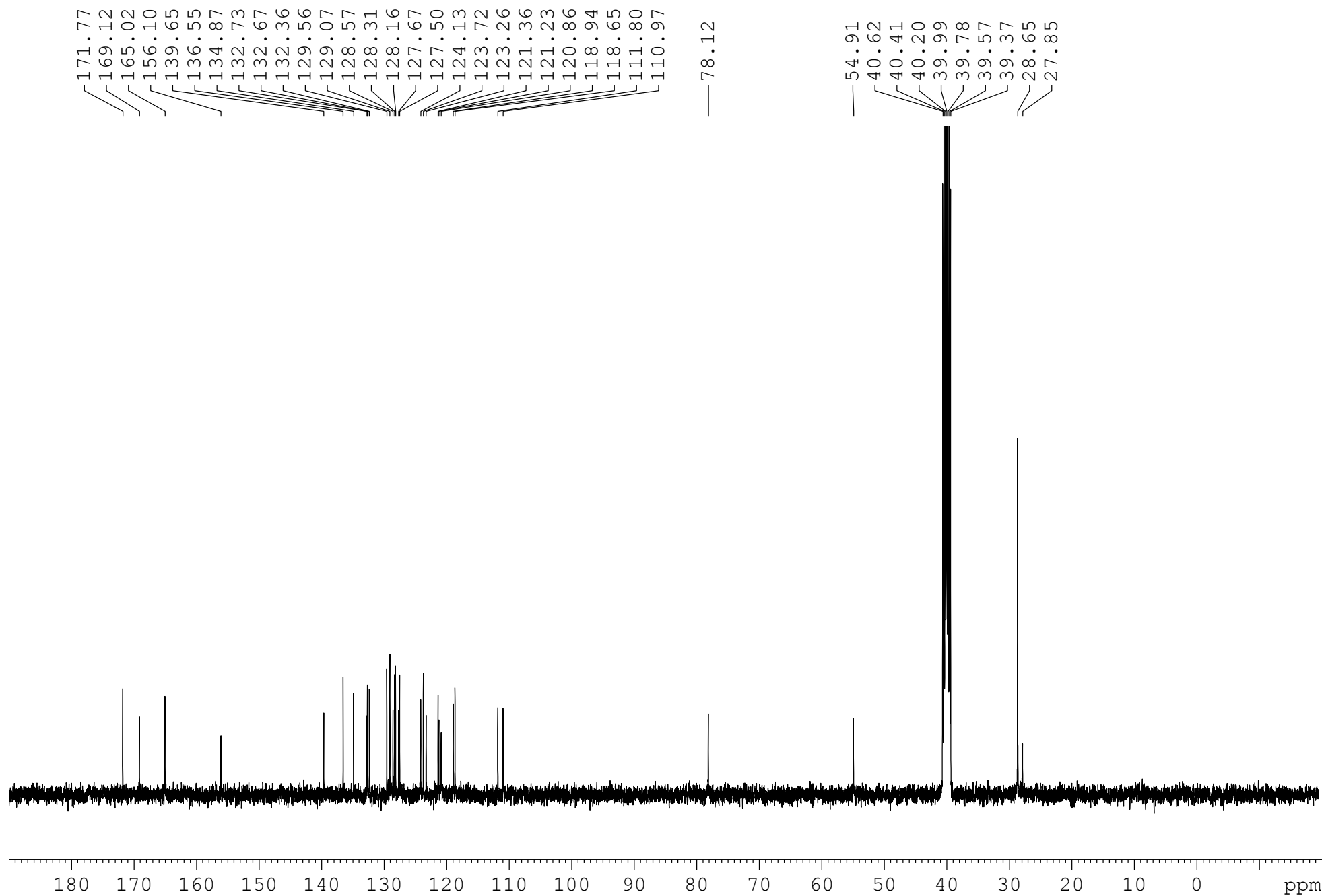
^{13}C NMR spectra of (2-(2-naphthamido)-5-methoxybenzoyl)-*L*-tryptophan (**4e**)



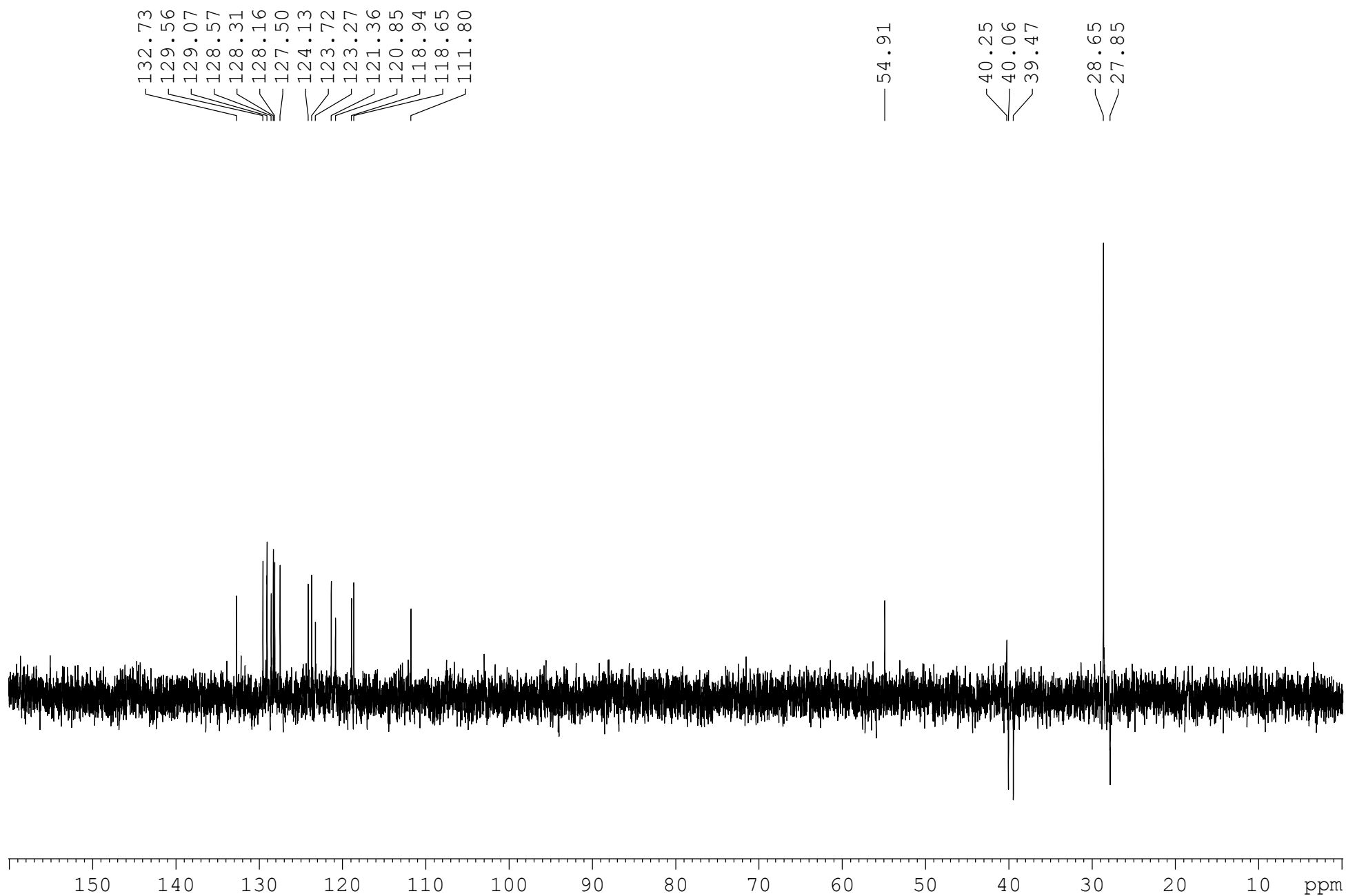
¹H NMR spectra of *tert*-butyl (*S*)-(2-(2-(2-(2-naphthamido)benzamido)-3-(1*H*-indol-3-yl)propanamido)ethyl)carbamate (**5a**)



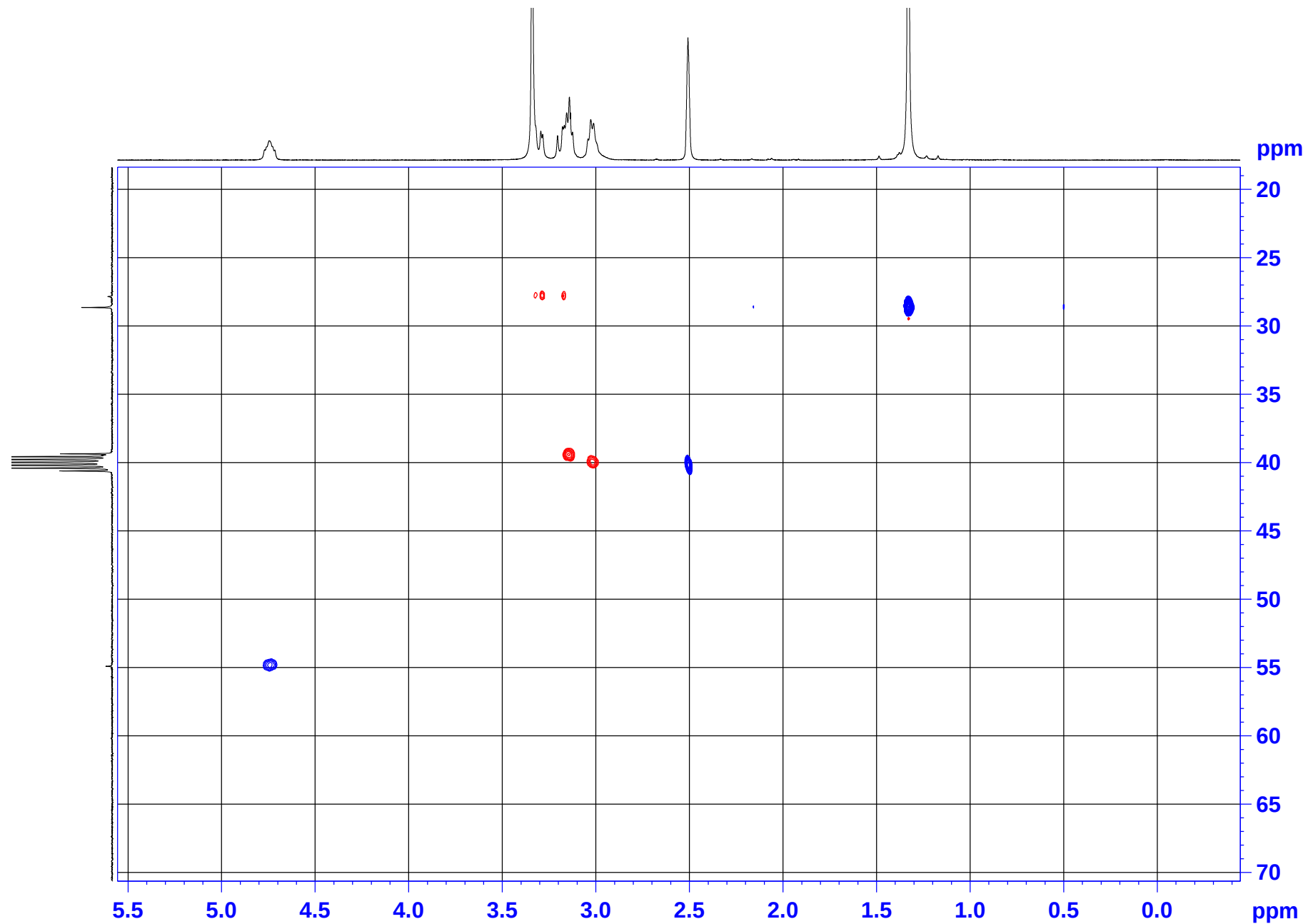
^{13}C NMR spectra of *tert*-butyl (*S*)-(2-(2-(2-(2-naphthamido)benzamido)-3-(1*H*-indol-3-yl)propanamido)ethyl)carbamate (**5a**)



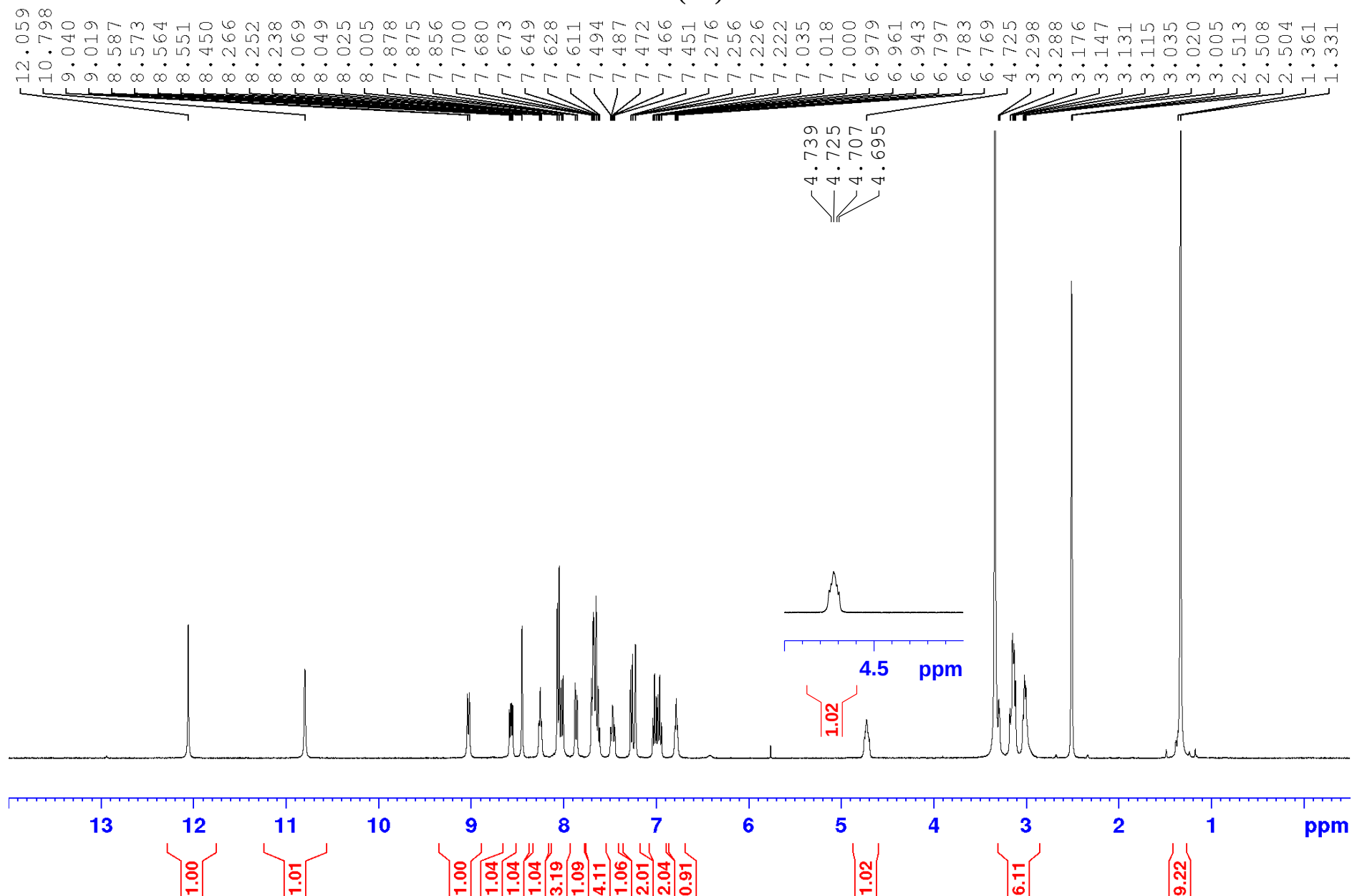
DEPT-135 NMR spectra of tert-butyl (S)-2-(2-(2-(2-naphthamido)benzamido)-3-(1H-indol-3-yl)propanamido)ethyl)carbamate (**5a**)



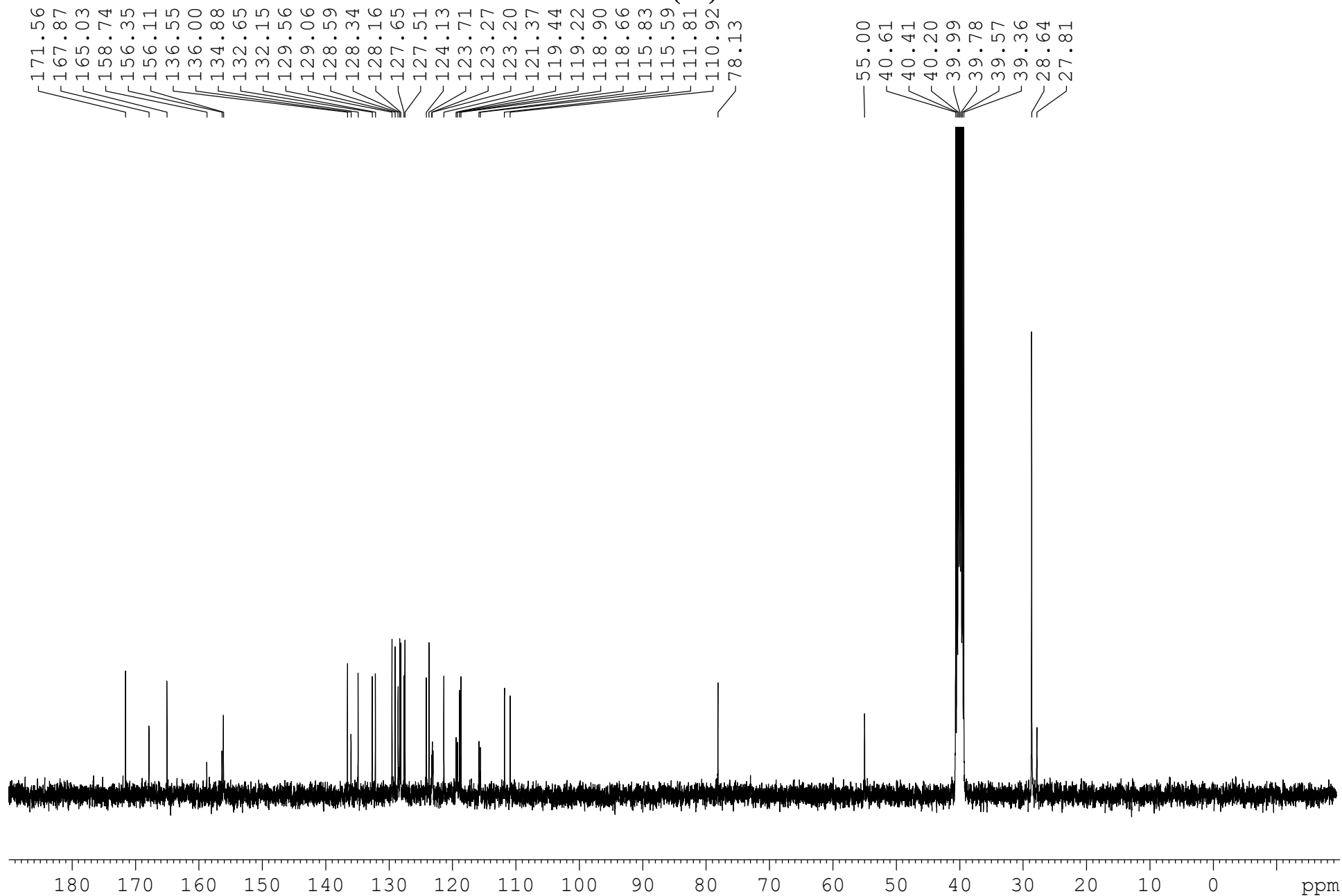
HSQC NMR spectra of tert-butyl (S)-2-(2-(2-(2-naphthamido)benzamido)-3-(1H-indol-3-yl)propanamido)ethyl)carbamate (**5a**)



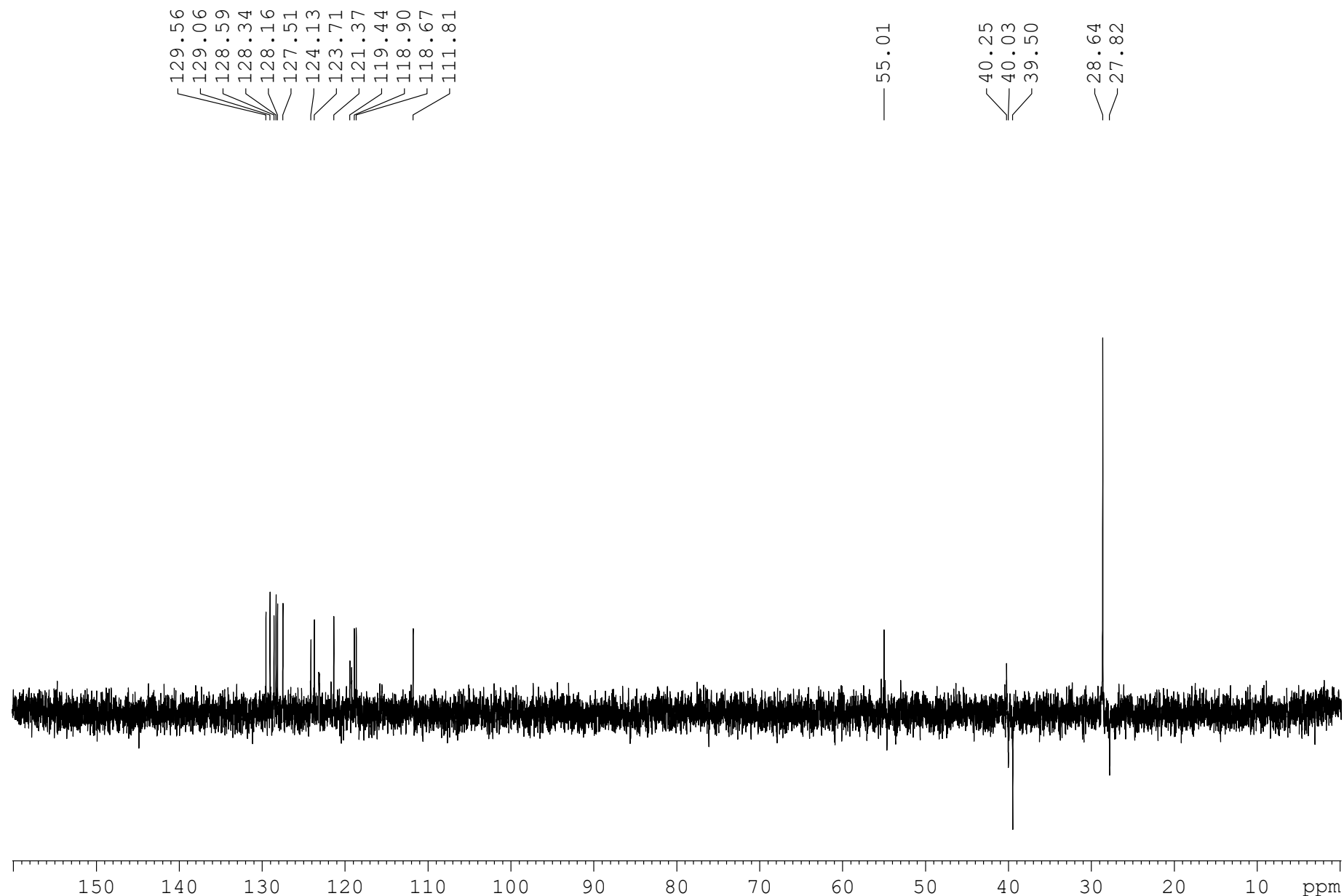
¹H NMR spectra of *tert*-butyl (*S*)-(2-(2-(2-(2-naphthamido)-5-fluorobenzamido)-3-(1H-indol-3-yl)propanamido)ethyl)carbamate (5b)



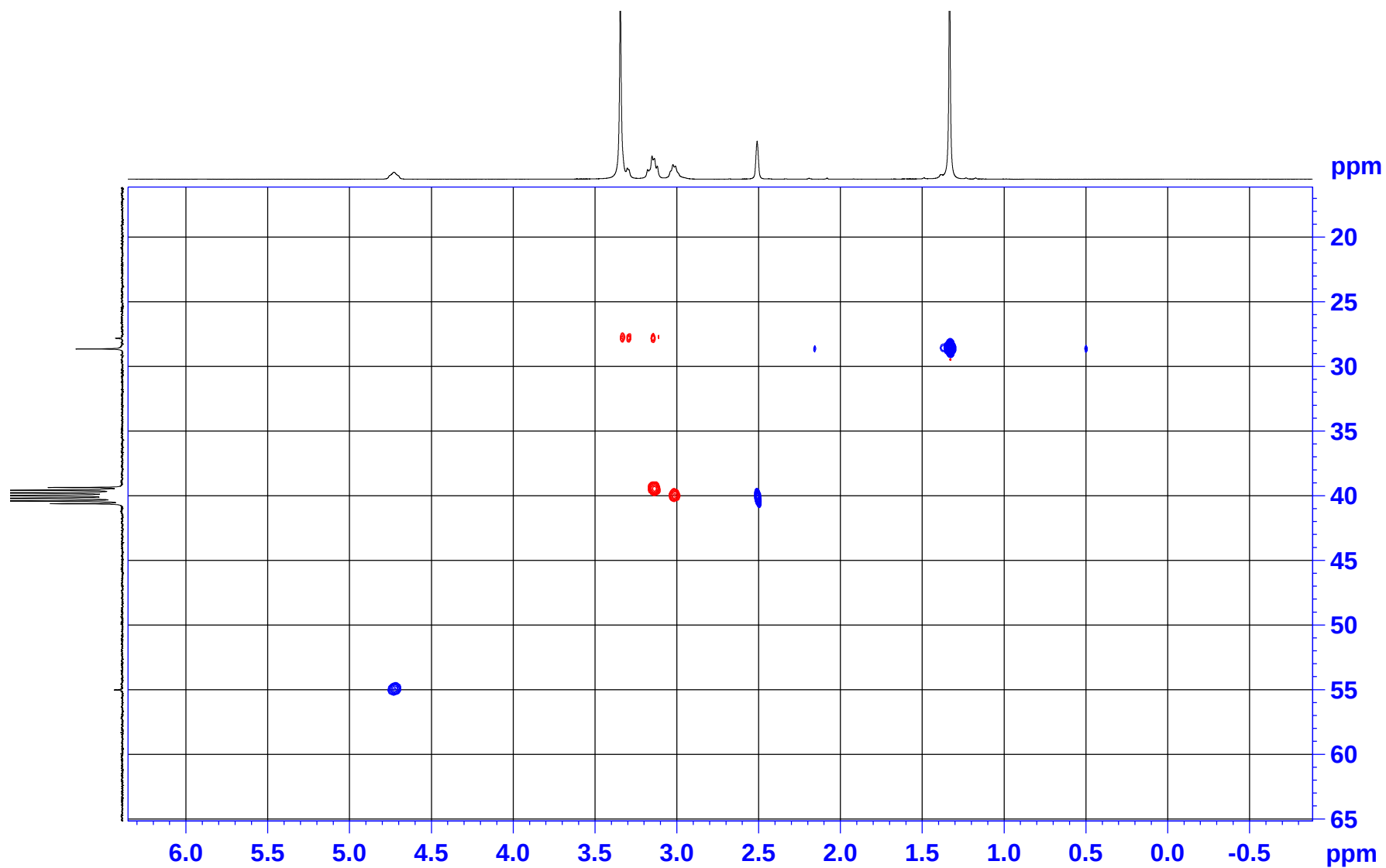
¹³C NMR spectra of *tert*-butyl (*S*)-(2-(2-(2-(2-naphthamido)-5-fluorobenzamido)-3-(1*H*-indol-3-yl)propanamido)ethyl)carbamate (5b)



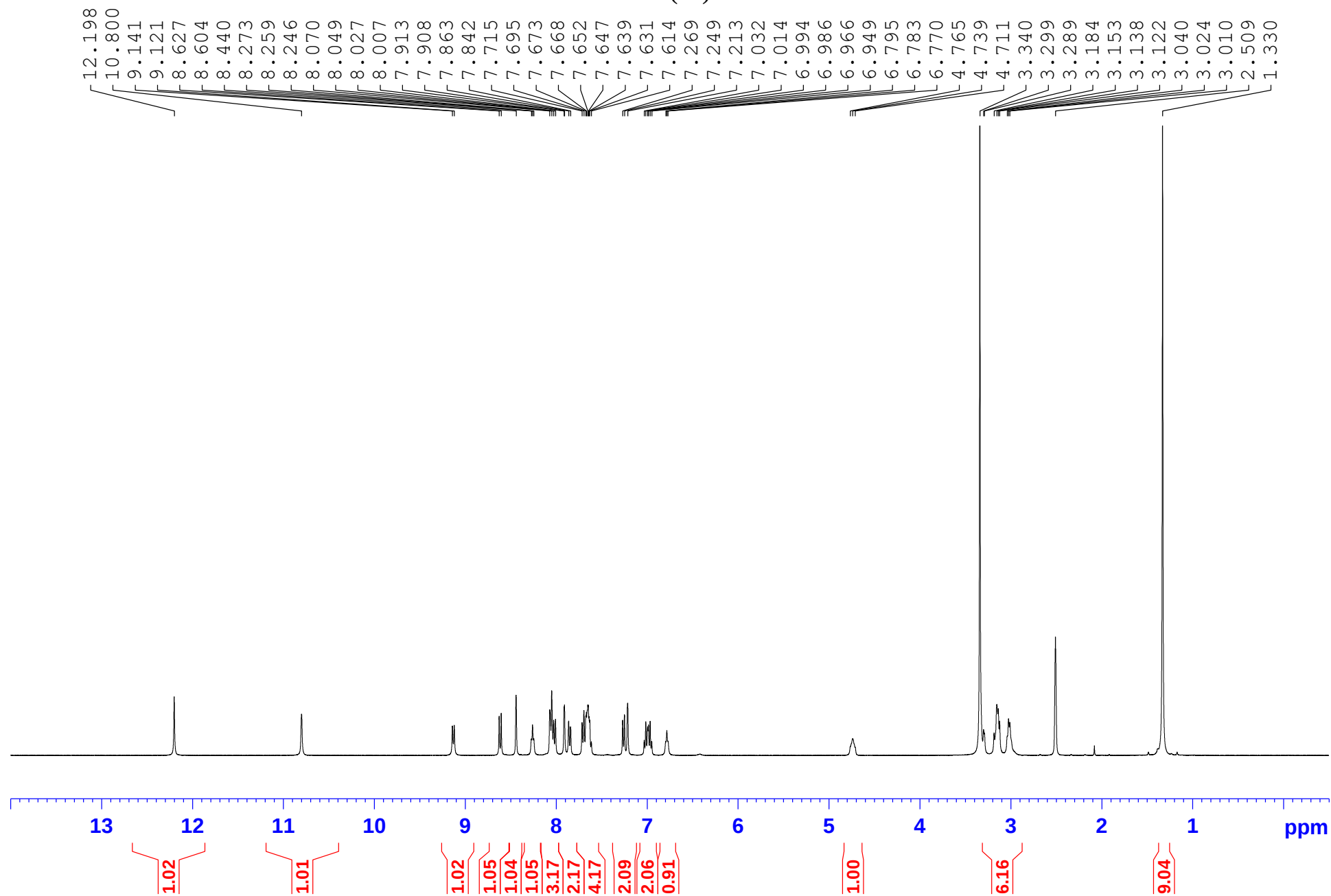
DEPT-135 NMR spectra of tert-butyl (S)-(2-(2-(2-(2-naphthamido)-5-fluorobenzamido)-3-(1H-indol-3-yl)propanamido)ethyl)carbamate (5b)



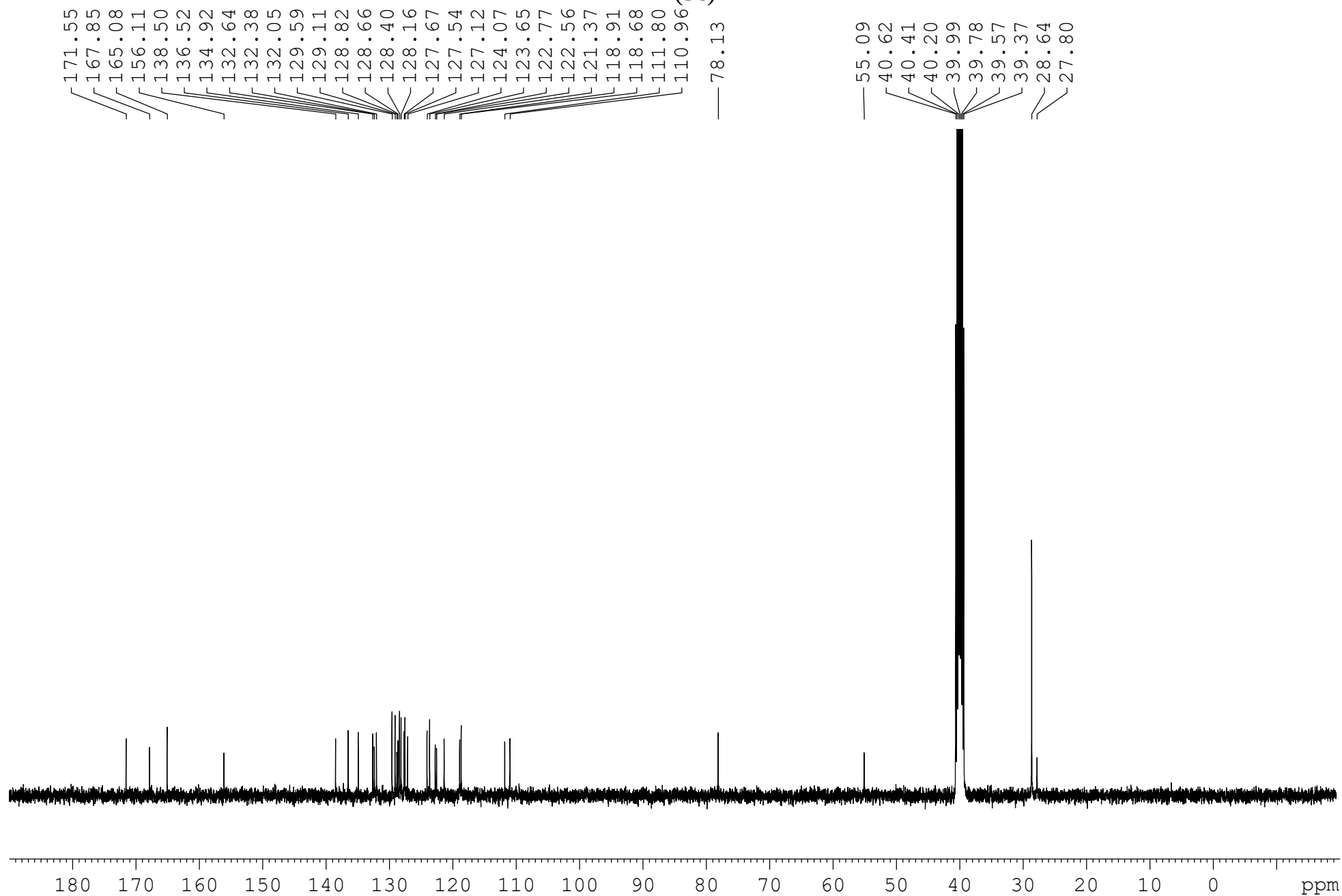
HSQC NMR spectra of tert-butyl (S)-(2-(2-(2-(2-naphthamido)-5-fluorobenzamido)-3-(1H-indol-3-yl)propanamido)ethyl)carbamate
(5b)



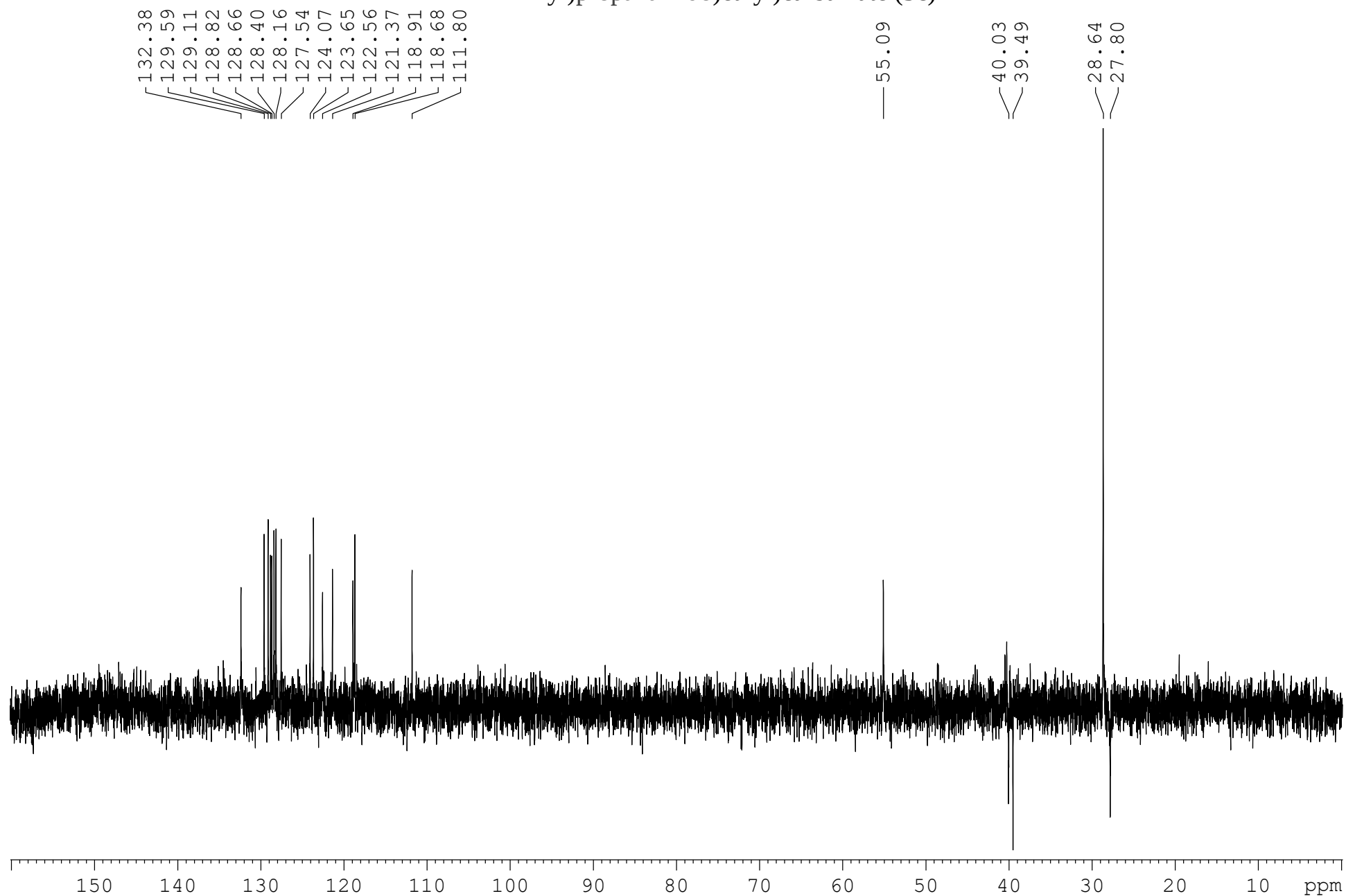
^1H NMR spectra of *tert*-butyl (S)-(2-(2-(2-(2-naphthamido)-5-chlorobenzamido)-3-(1*H*-indol-3-yl)propanamido)ethyl)carbamate (5c)



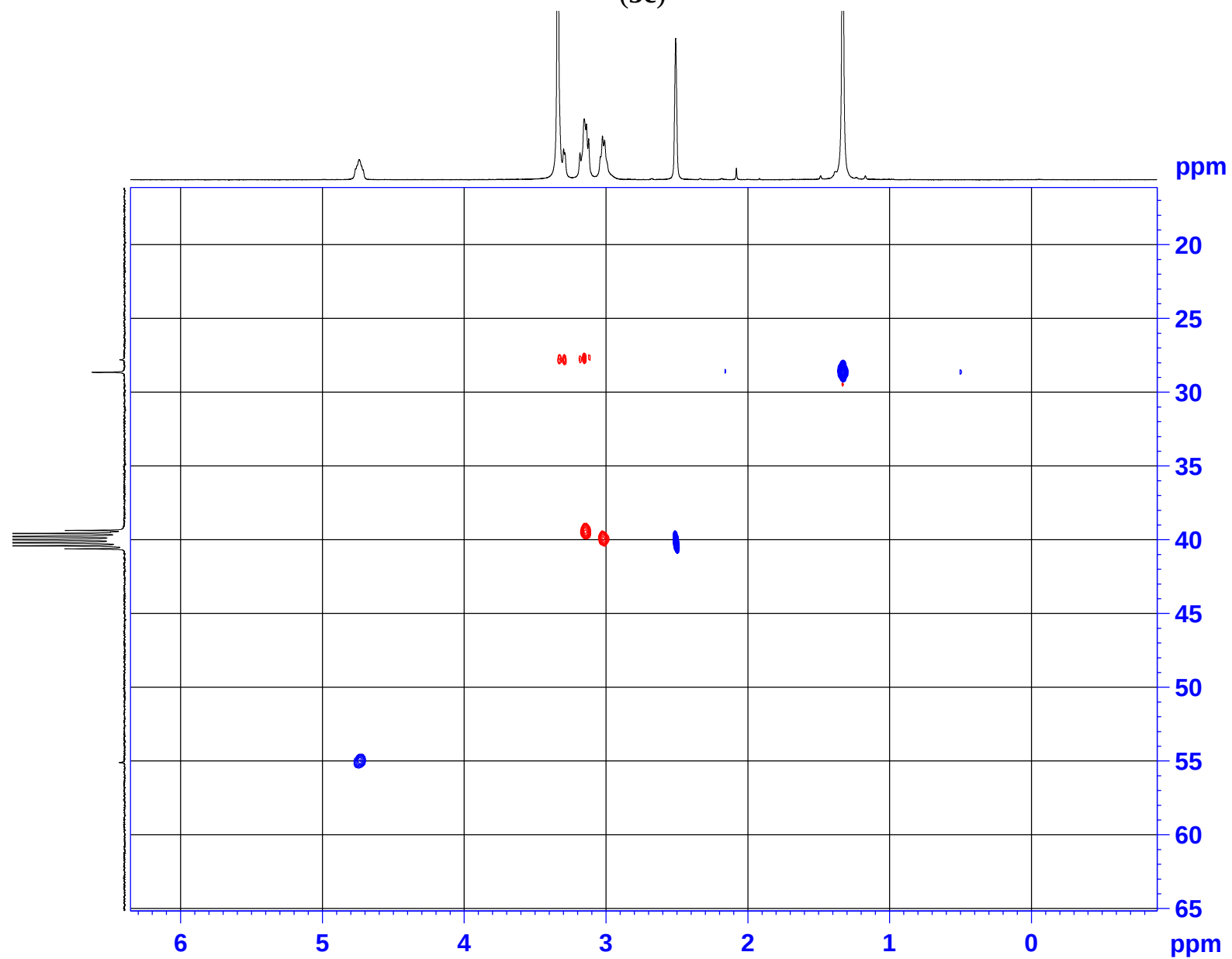
^{13}C NMR spectra of *tert*-butyl (*S*)-(2-(2-(2-(2-naphthamido)-5-chlorobenzamido)-3-(1*H*-indol-3-yl)propanamido)ethyl)carbamate (5c)



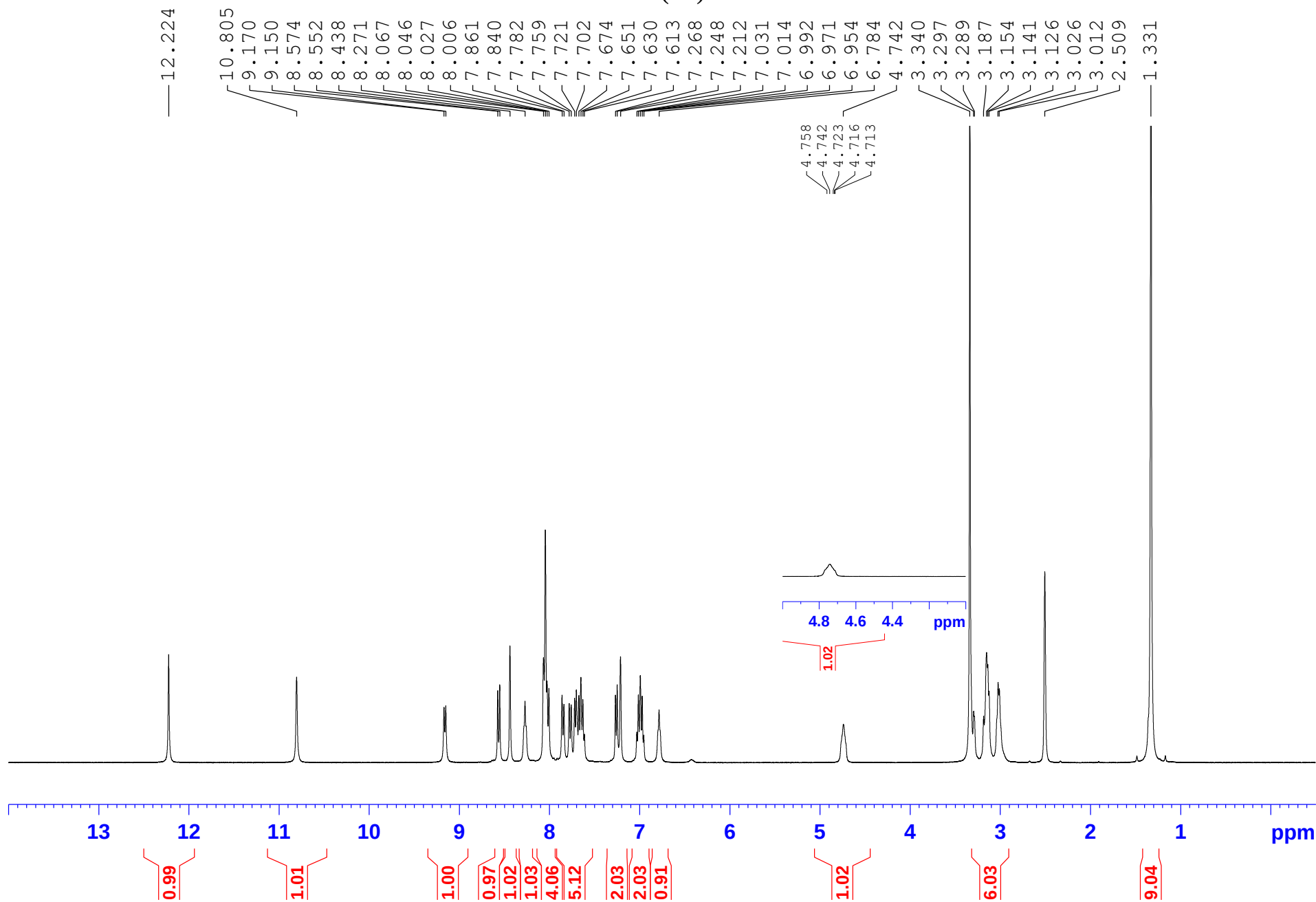
DEPT-135 NMR spectra of *tert*-butyl (*S*)-(2-(2-(2-(2-naphthamido)-5-chlorobenzamido)-3-(1*H*-indol-3-yl)propanamido)ethyl)carbamate (**5c**)



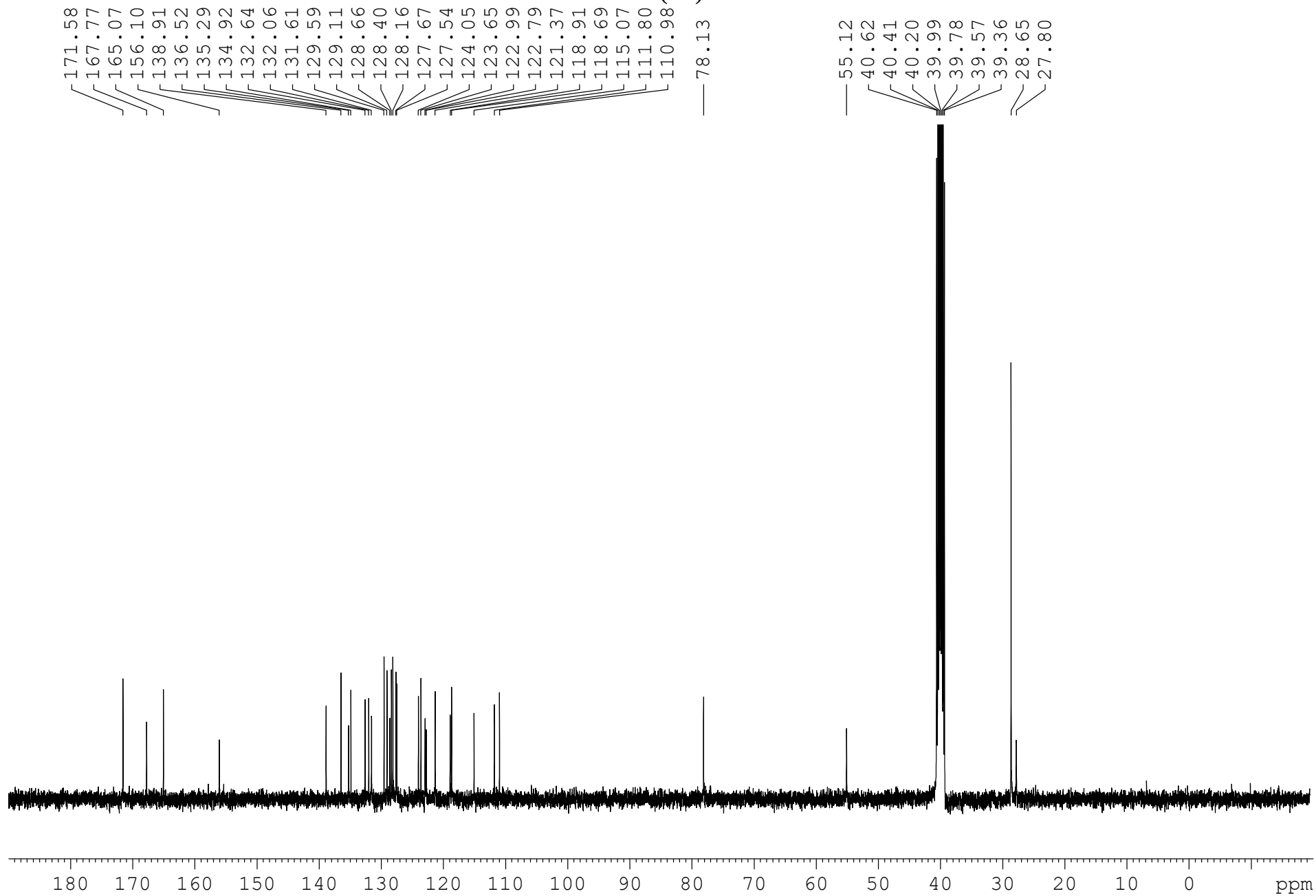
HSQC NMR spectra of *tert*-butyl (*S*)-(2-(2-(2-(2-naphthamido)-5-chlorobenzamido)-3-(1*H*-indol-3-yl)propanamido)ethyl)carbamate (5c)



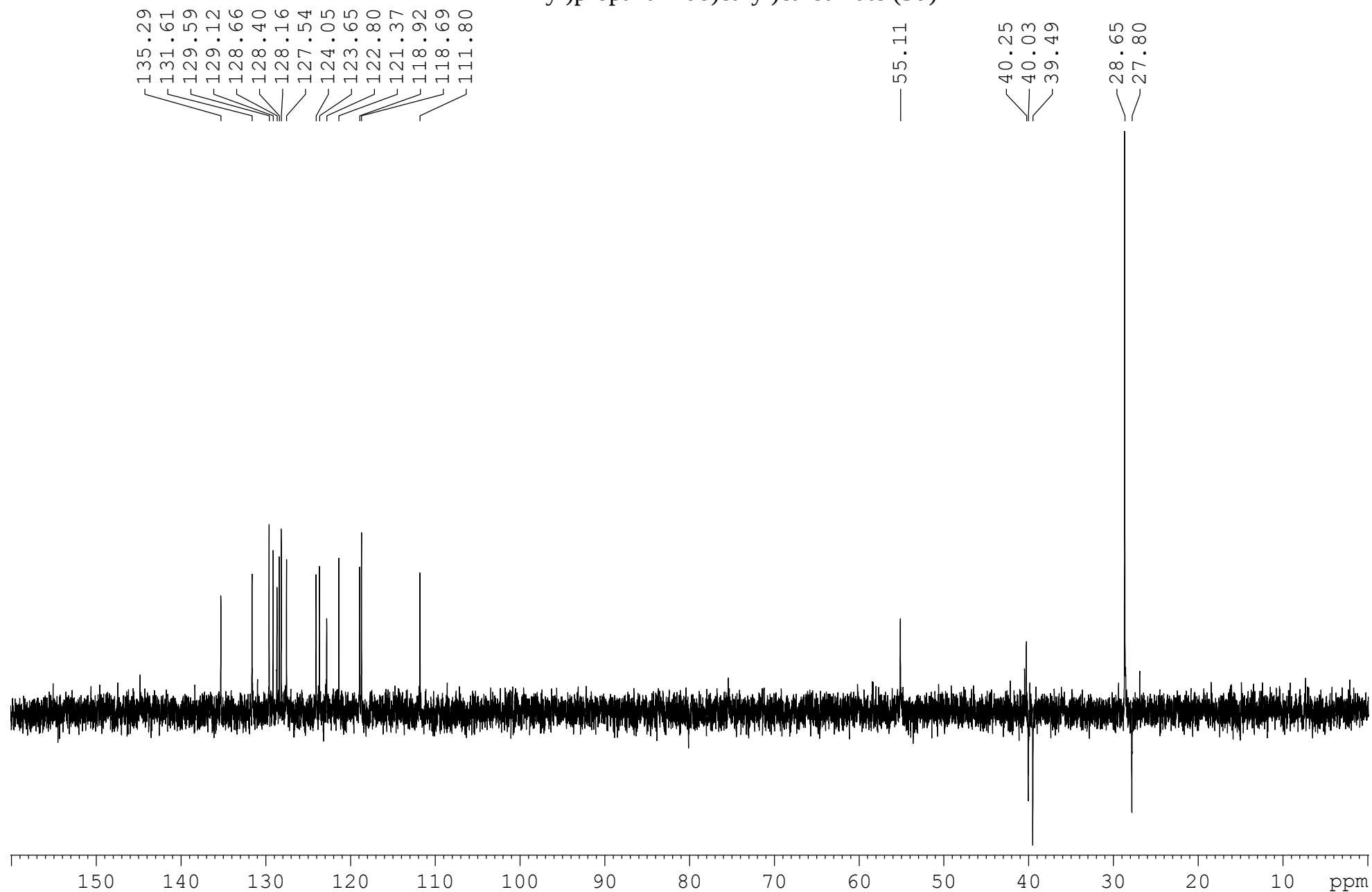
¹H NMR spectra of *tert*-butyl (S)-(2-(2-(2-(2-naphthamido)-5-bromobenzamido)-3-(1H-indol-3-yl)propanamido)ethyl)carbamate (5d)



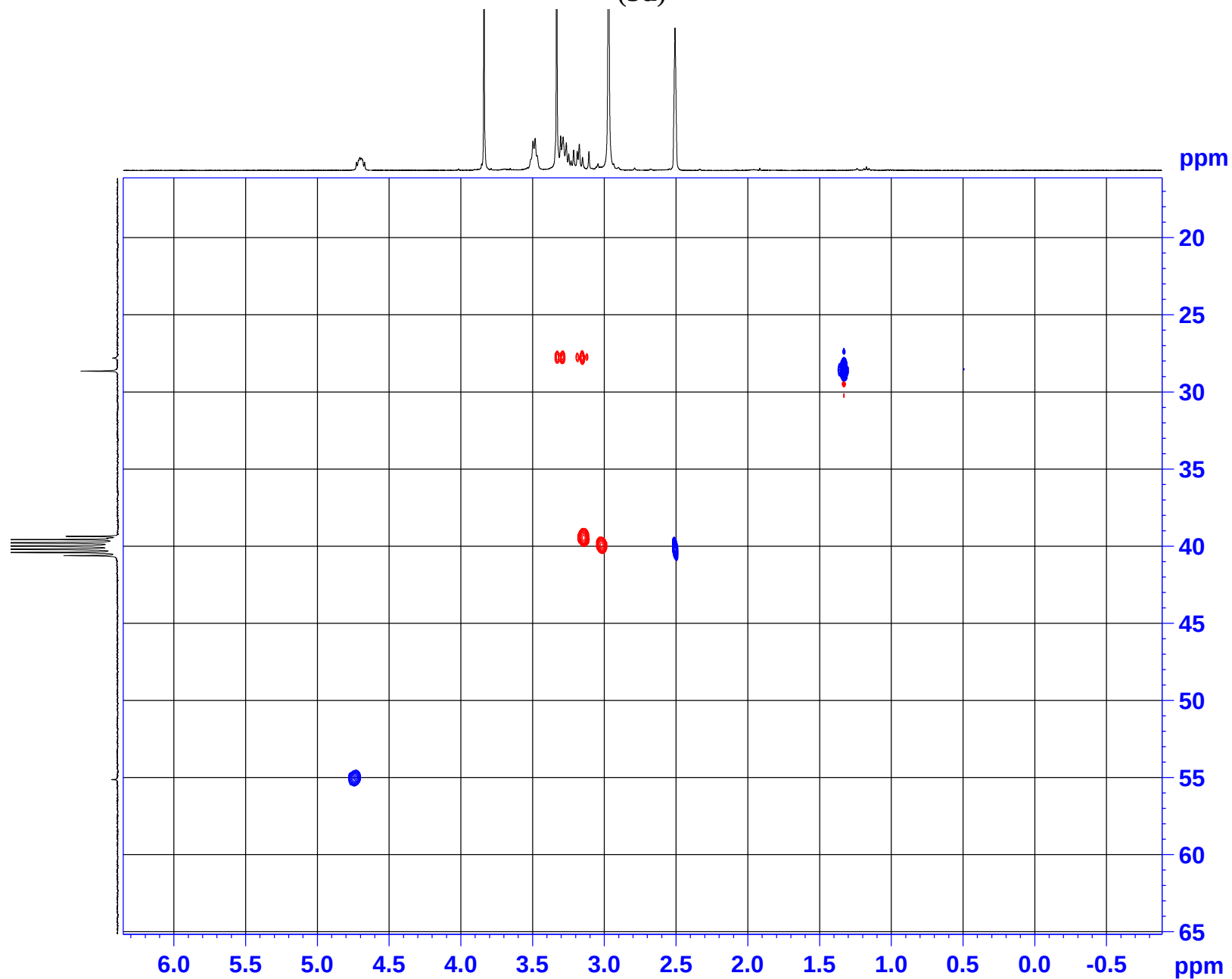
^{13}C NMR spectra of *tert*-butyl (*S*)-(2-(2-(2-(2-naphthamido)-5-bromobenzamido)-3-(1H-indol-3-yl)propanamido)ethyl)carbamate (5d)



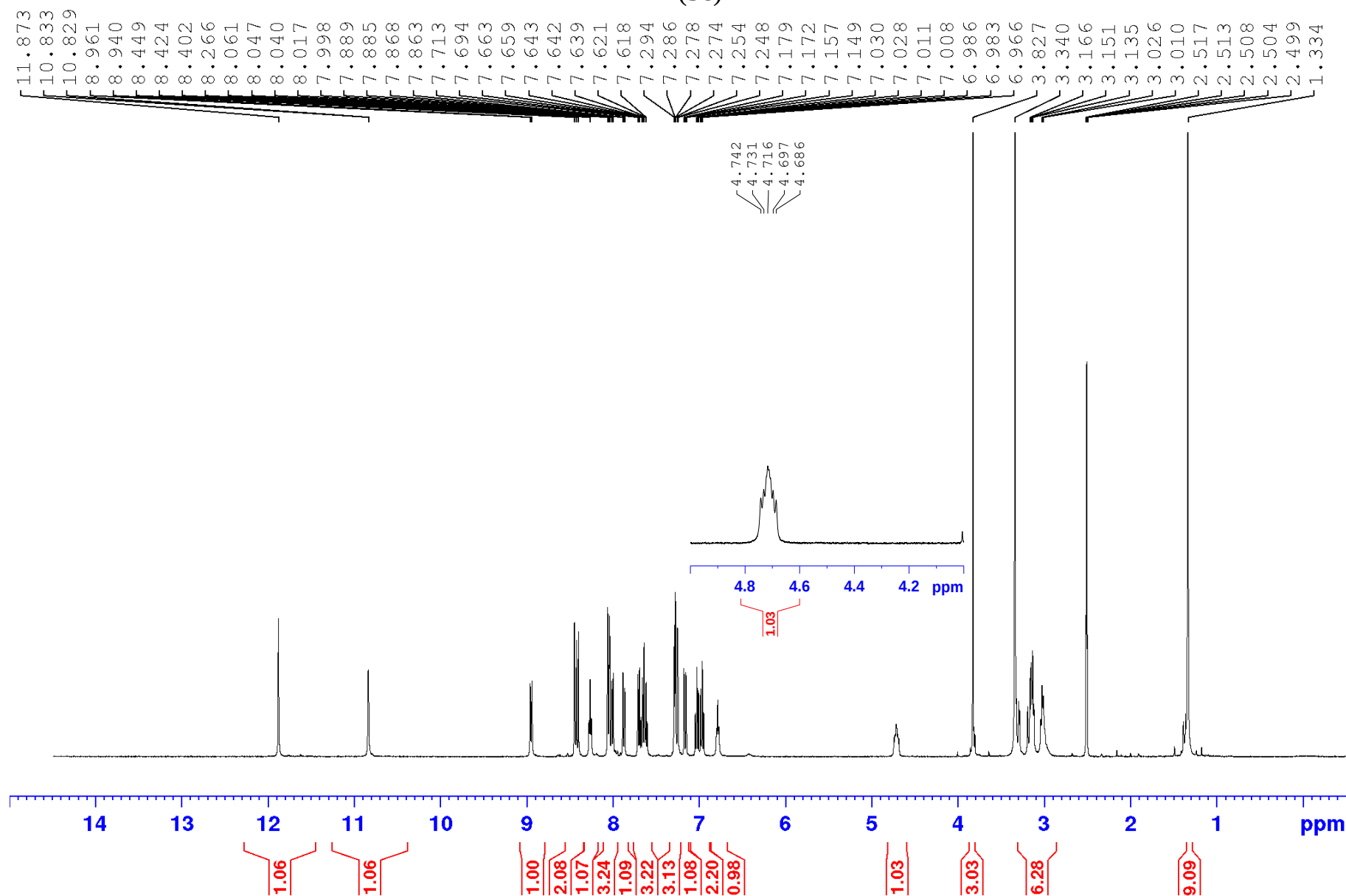
DEPT-135 NMR spectra of *tert*-butyl (*S*)-(2-(2-(2-(2-naphthamido)-5-bromobenzamido)-3-(1H-indol-3-yl)propanamido)ethyl)carbamate (**5d**)



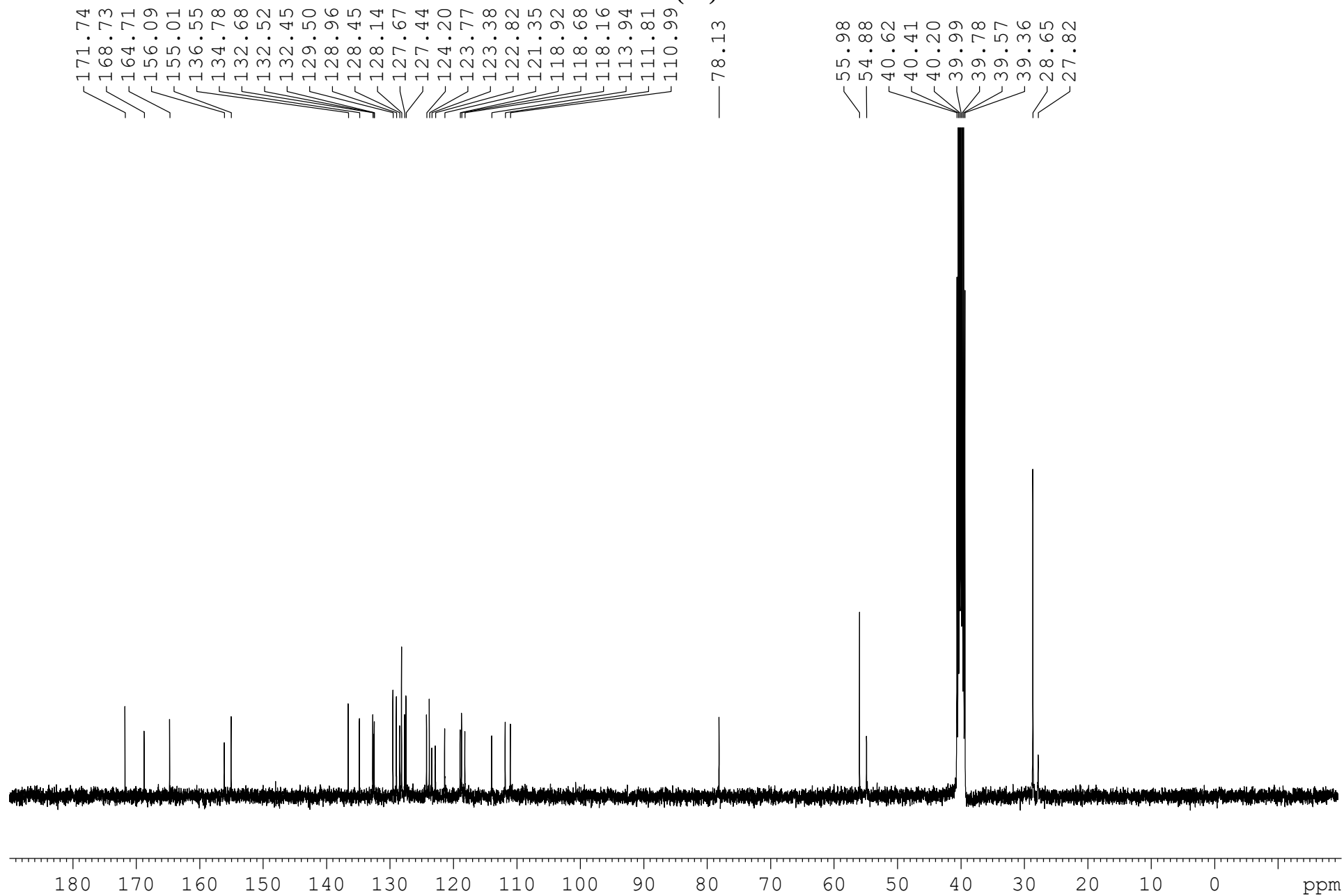
HSQC NMR spectra of *tert*-butyl (*S*)-(2-(2-(2-(2-naphthamido)-5-bromobenzamido)-3-(1H-indol-3-yl)propanamido)ethyl)carbamate
(5d)



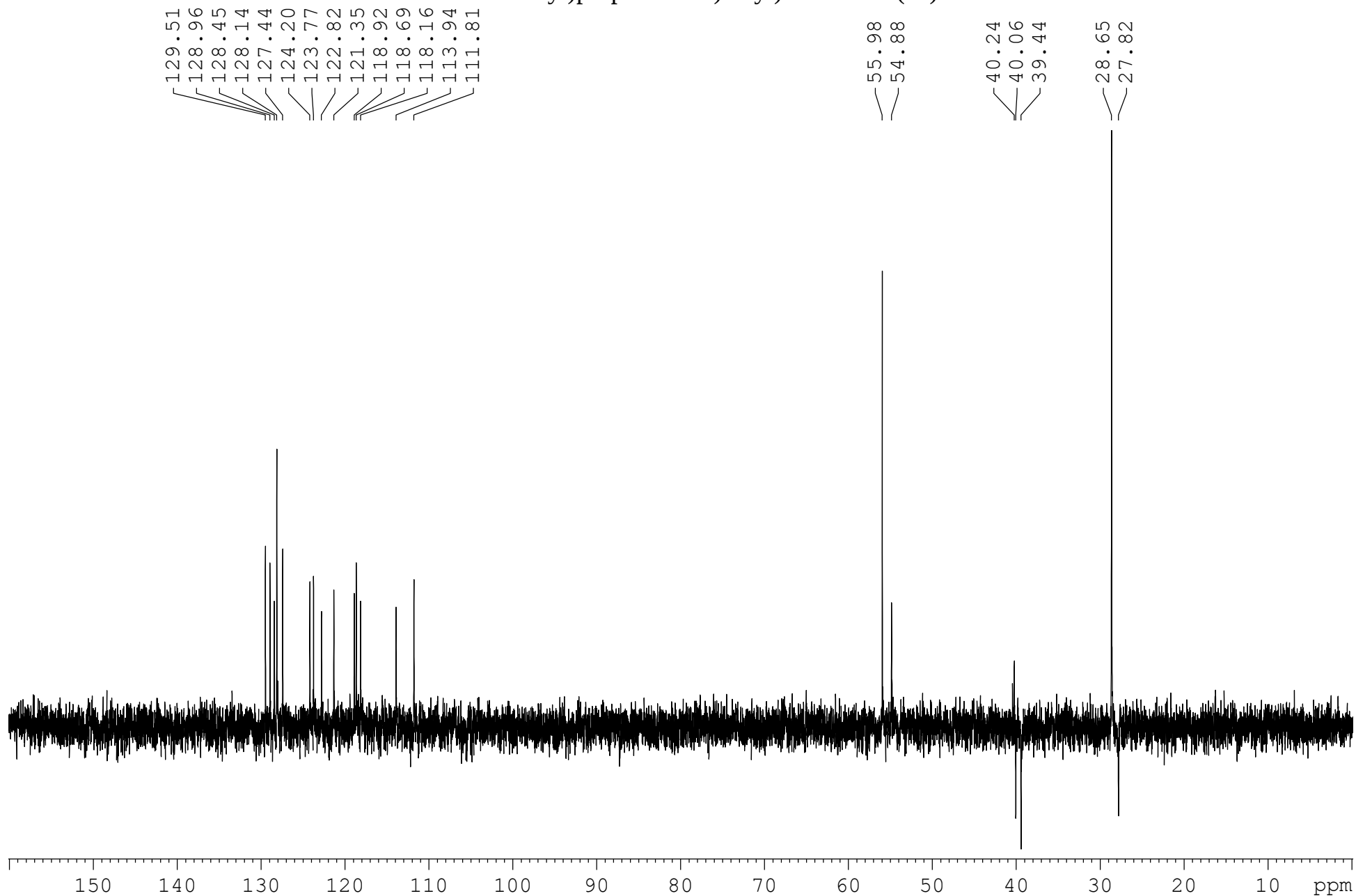
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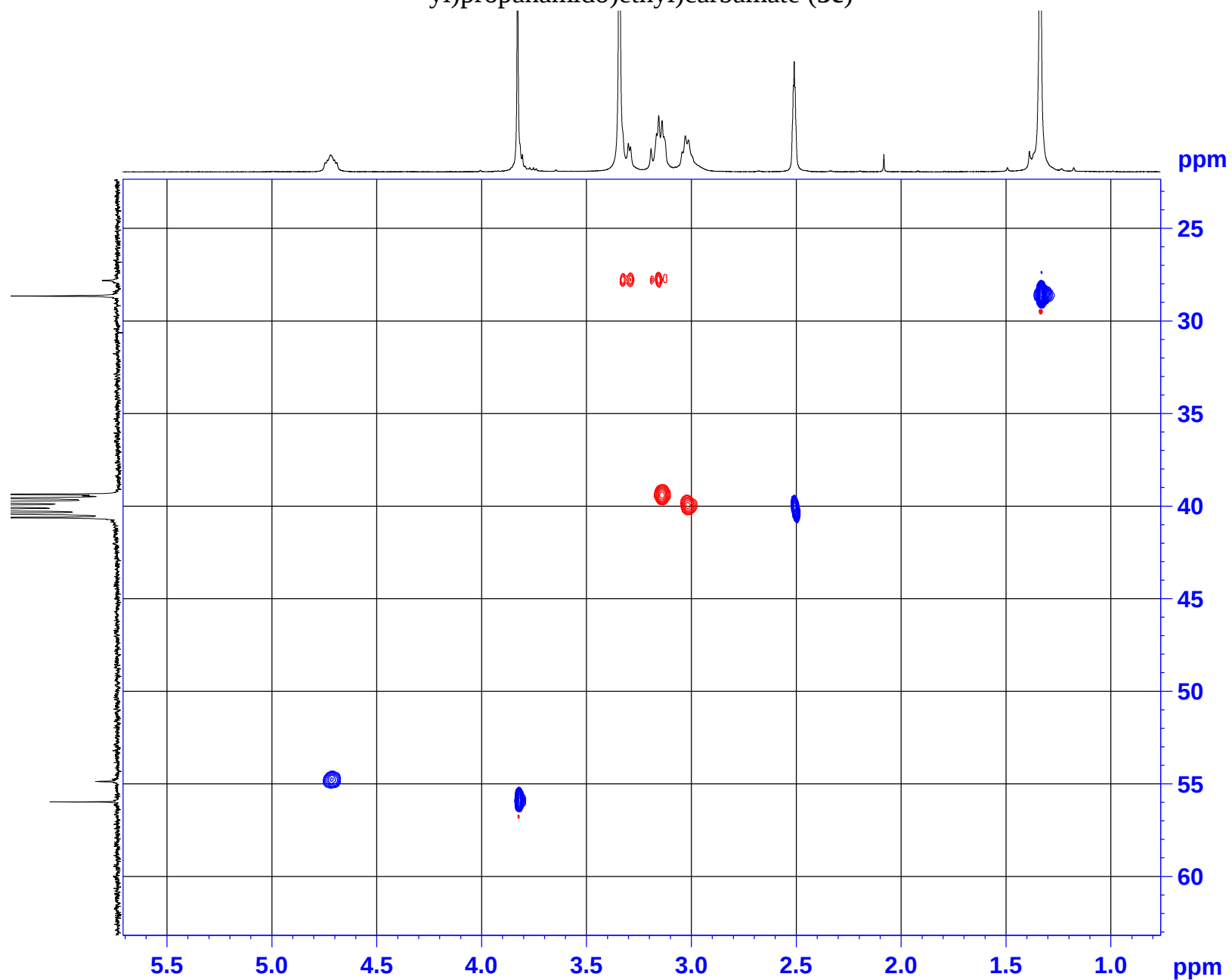
^{13}C NMR spectra of *tert*-butyl (*S*)-(2-(2-(2-(2-naphthamido)-5-methoxybenzamido)-3-(1H-indol-3-yl)propanamido)ethyl)carbamate (5e)



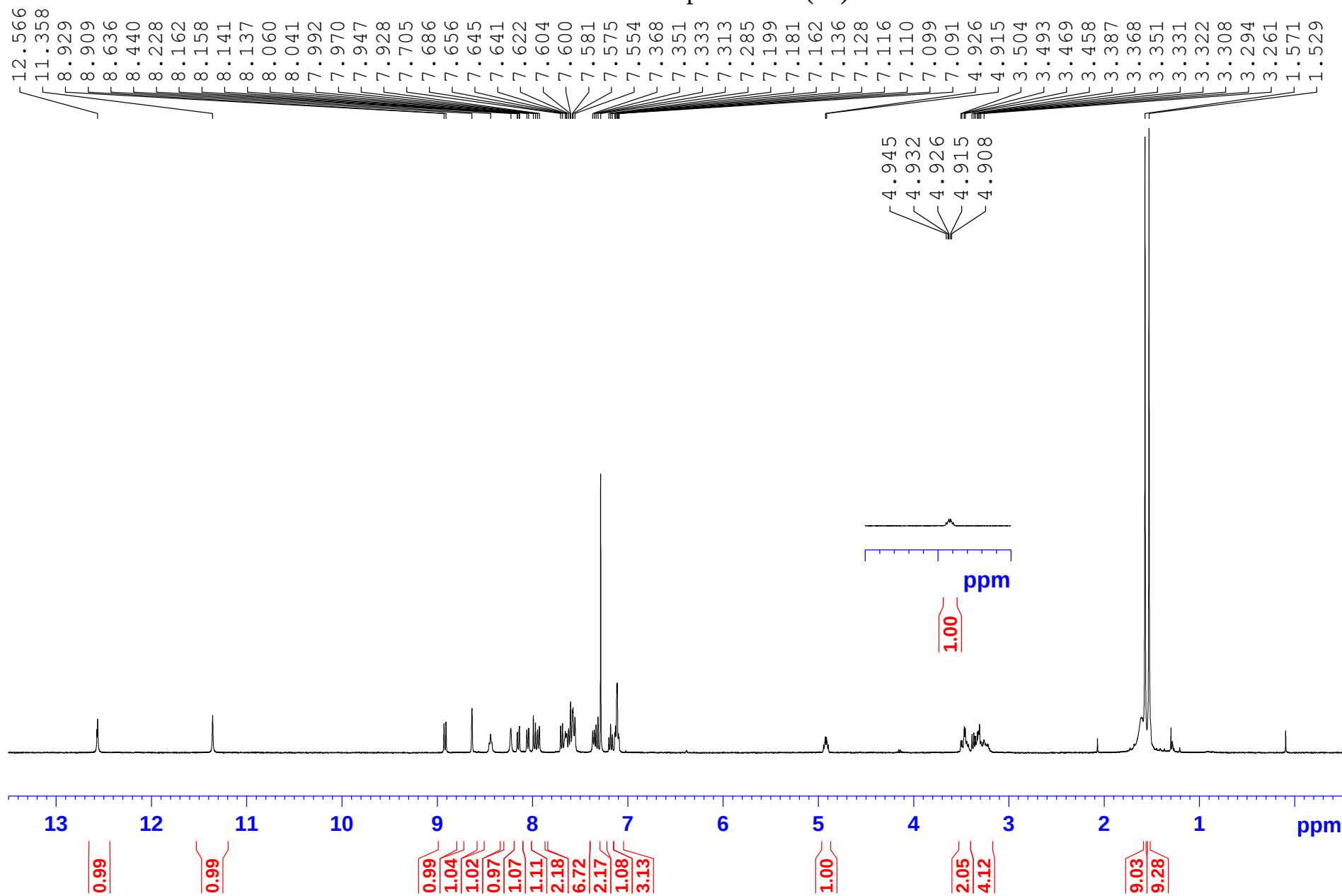
DEPT-135 NMR spectra of *tert*-butyl (*S*)-(2-(2-(2-(2-naphthamido)-5-methoxybenzamido)-3-(1H-indol-3-yl)propanamido)ethyl)carbamate (**5e**)



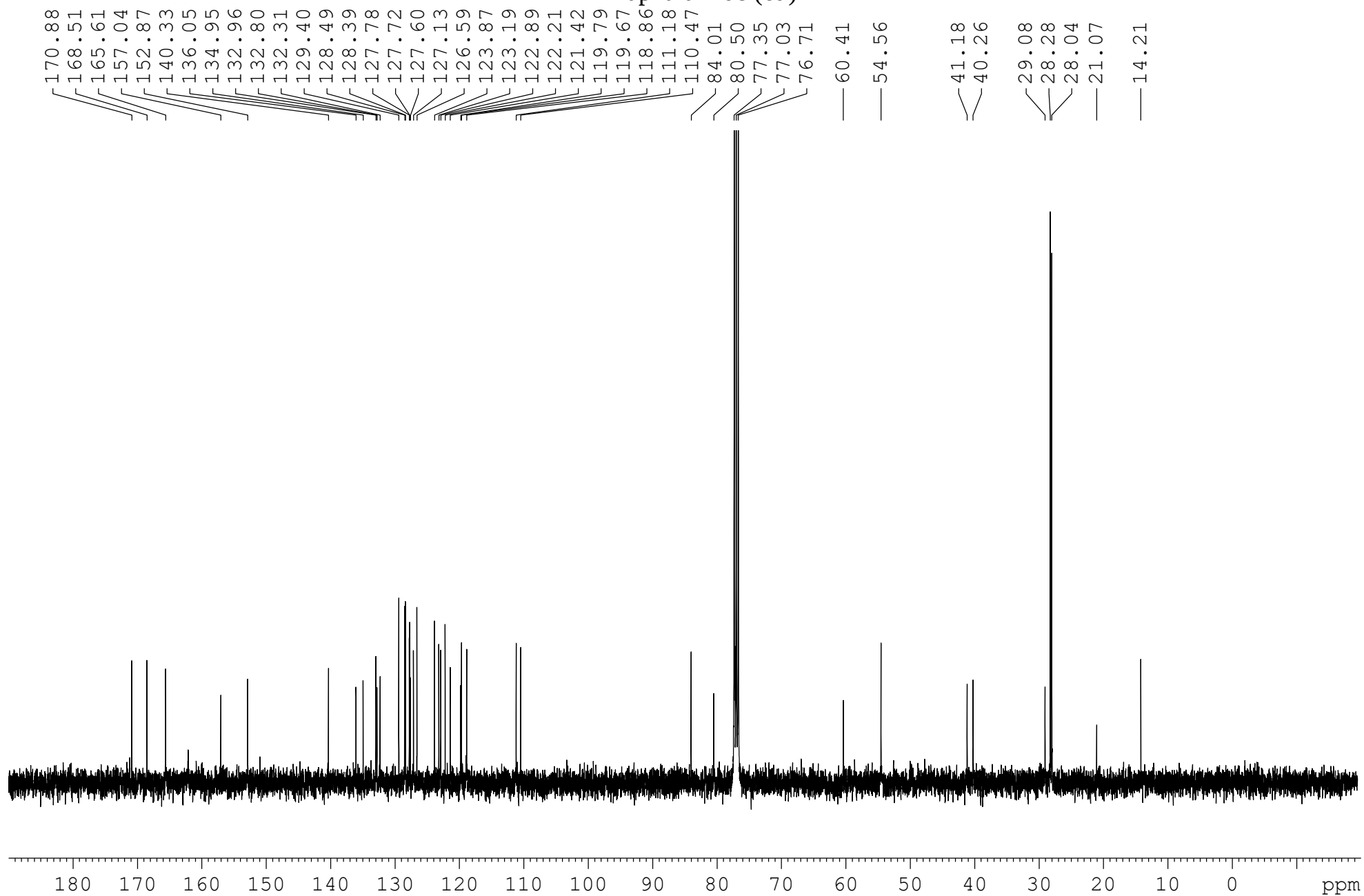
. HSQC NMR spectra of *tert*-butyl (*S*)-(2-(2-(2-(2-naphthamido)-5-methoxybenzamido)-3-(1H-indol-3-yl)propanamido)ethyl)carbamate (**5e**)



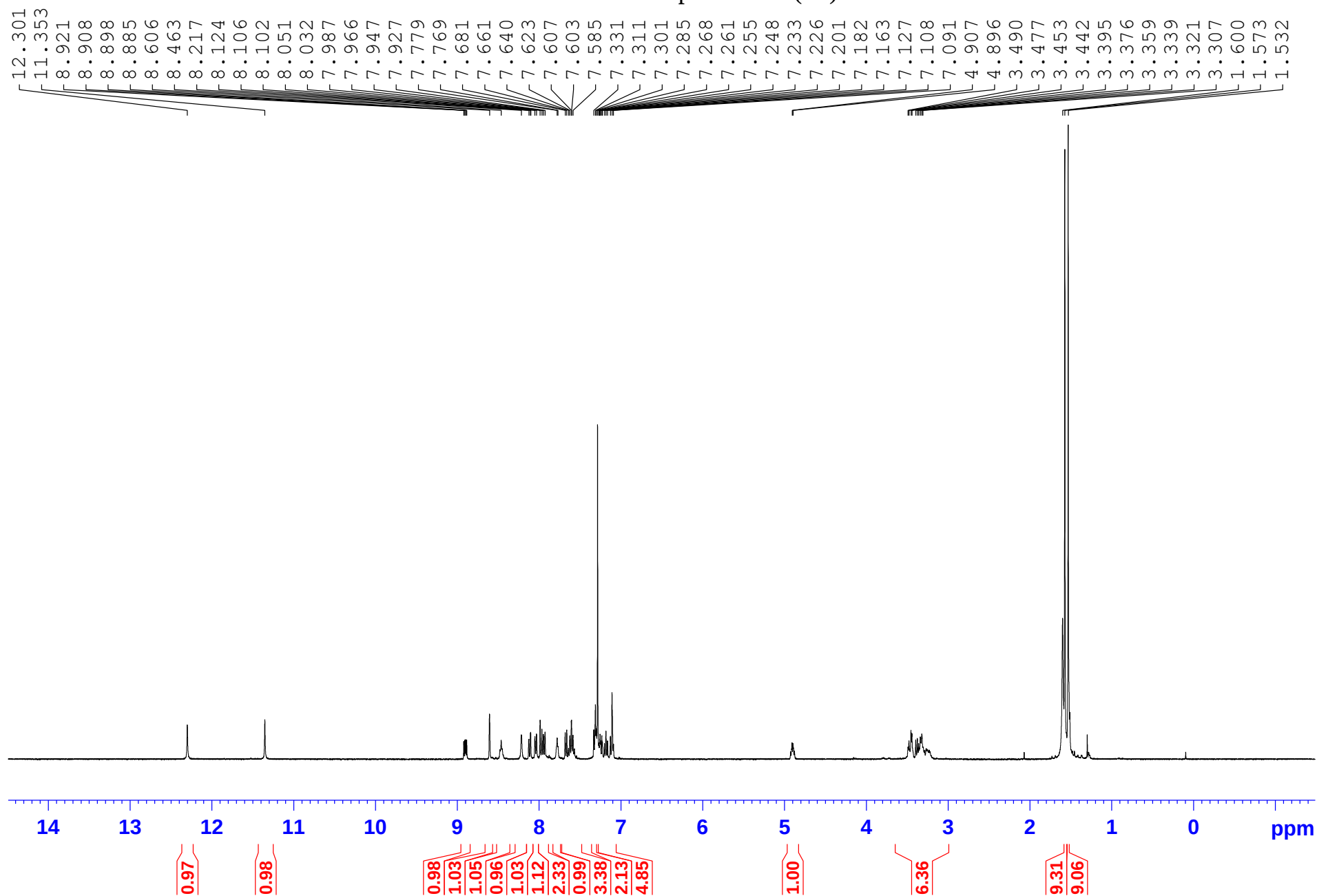
¹H NMR spectra of (S)-N-(2-((1-((2-diBocguanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (6a)



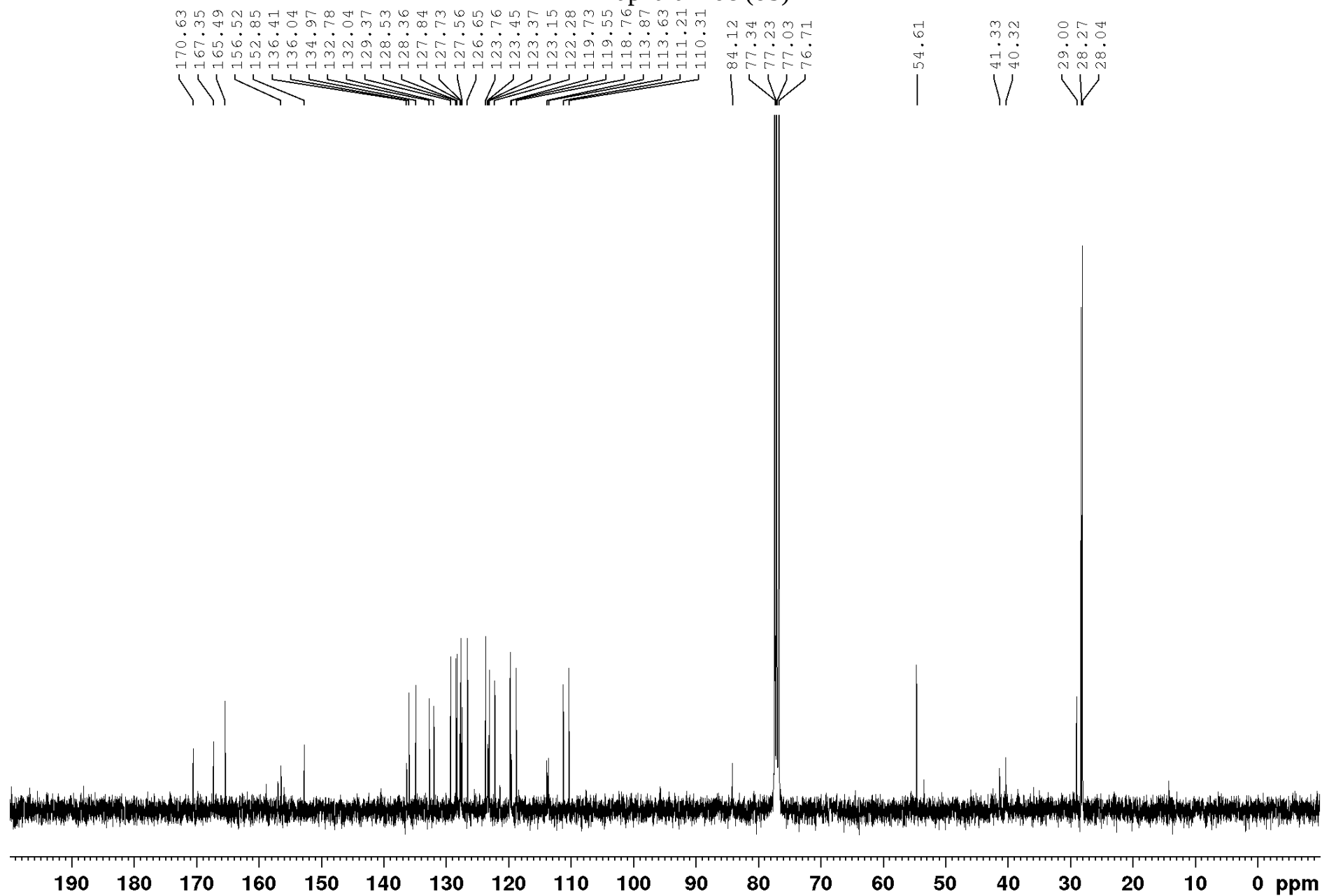
^{13}C NMR spectra of (S)-N-(2-((1-((2-diBocguanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (6a)



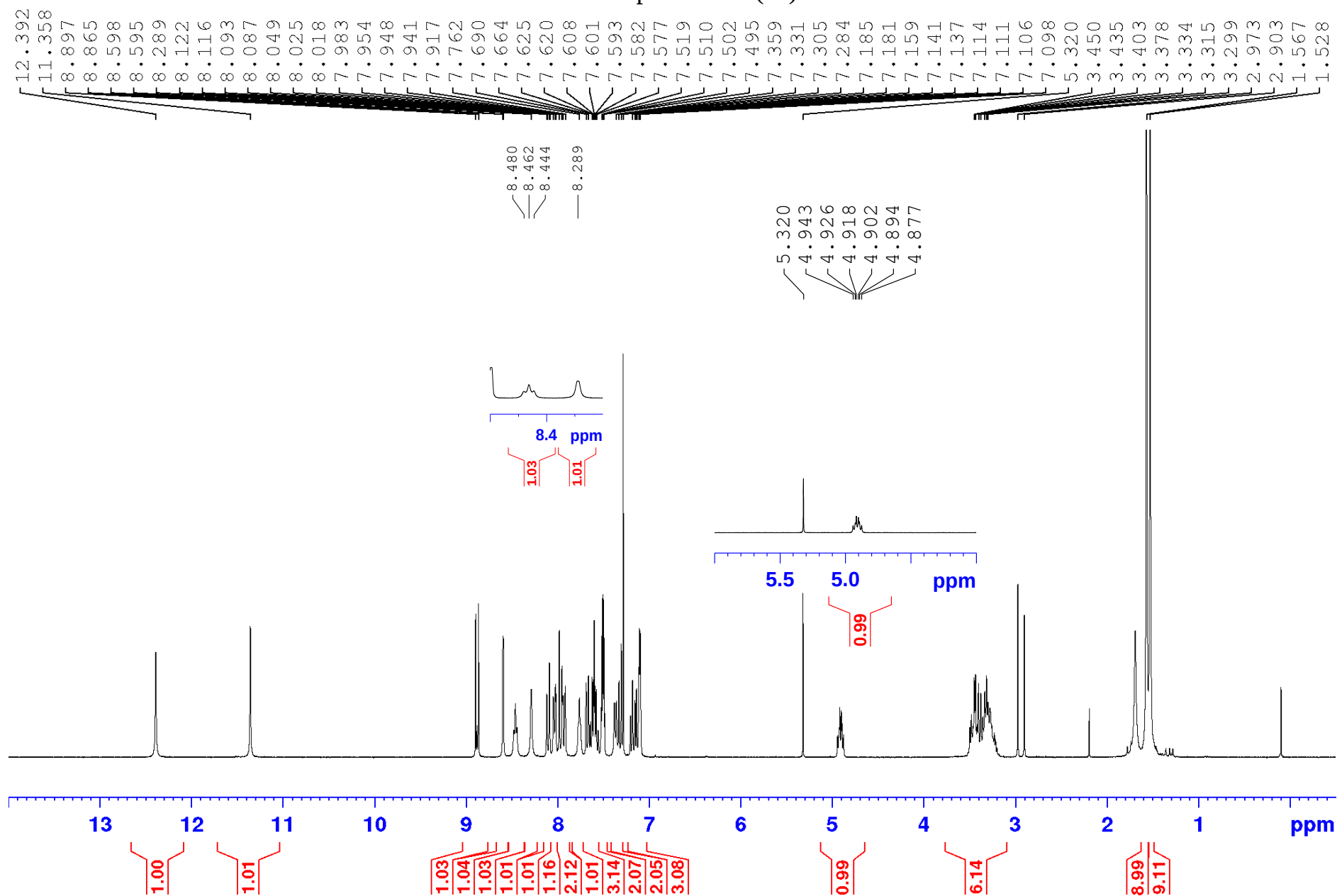
¹H NMR spectra of (S)-N-(4-fluoro-2-((1-((2-diBocguanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**6b**)



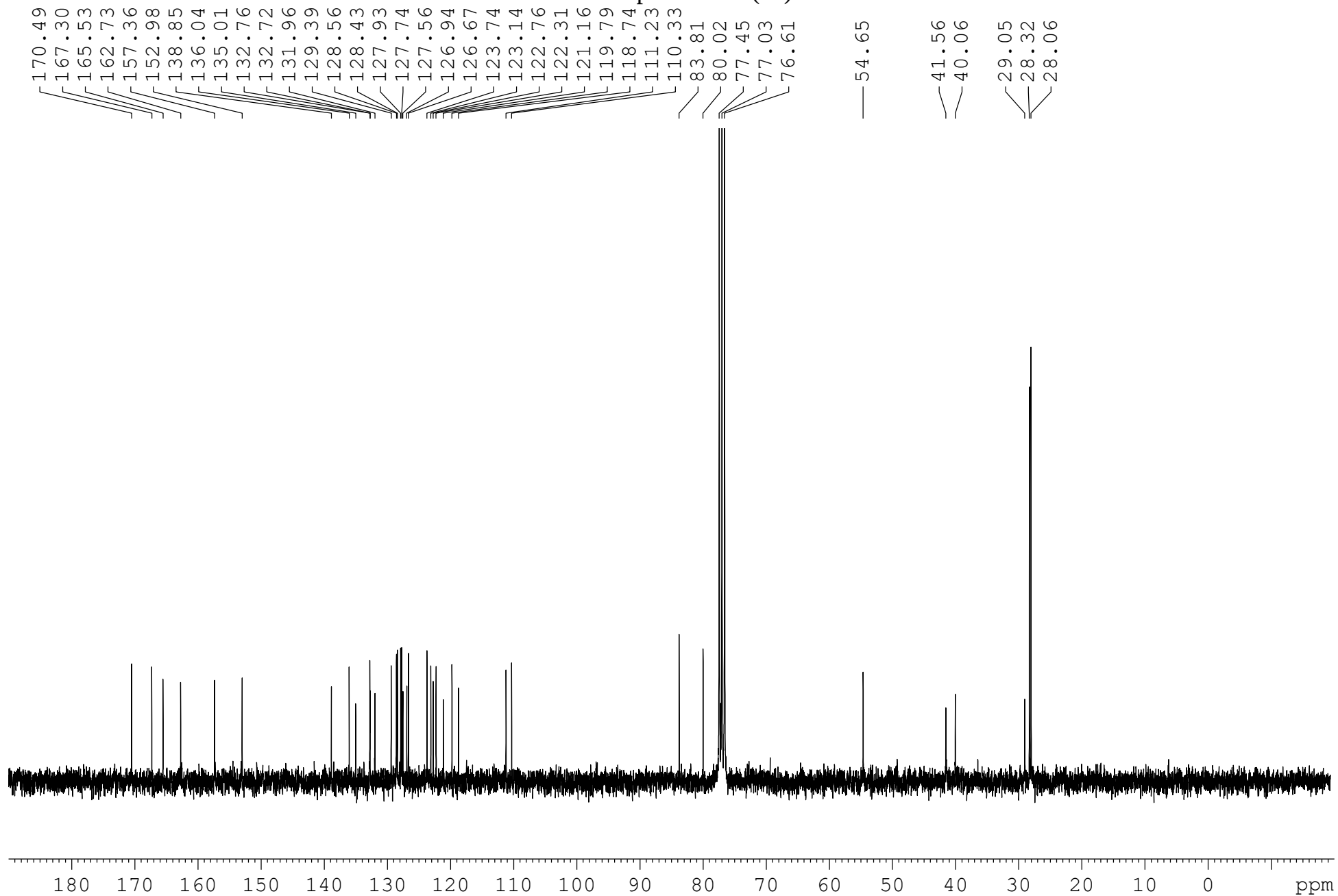
^{13}C NMR spectra of (*S*)-*N*-(4-fluoro-2-((1-((2-diBocguanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**6b**)

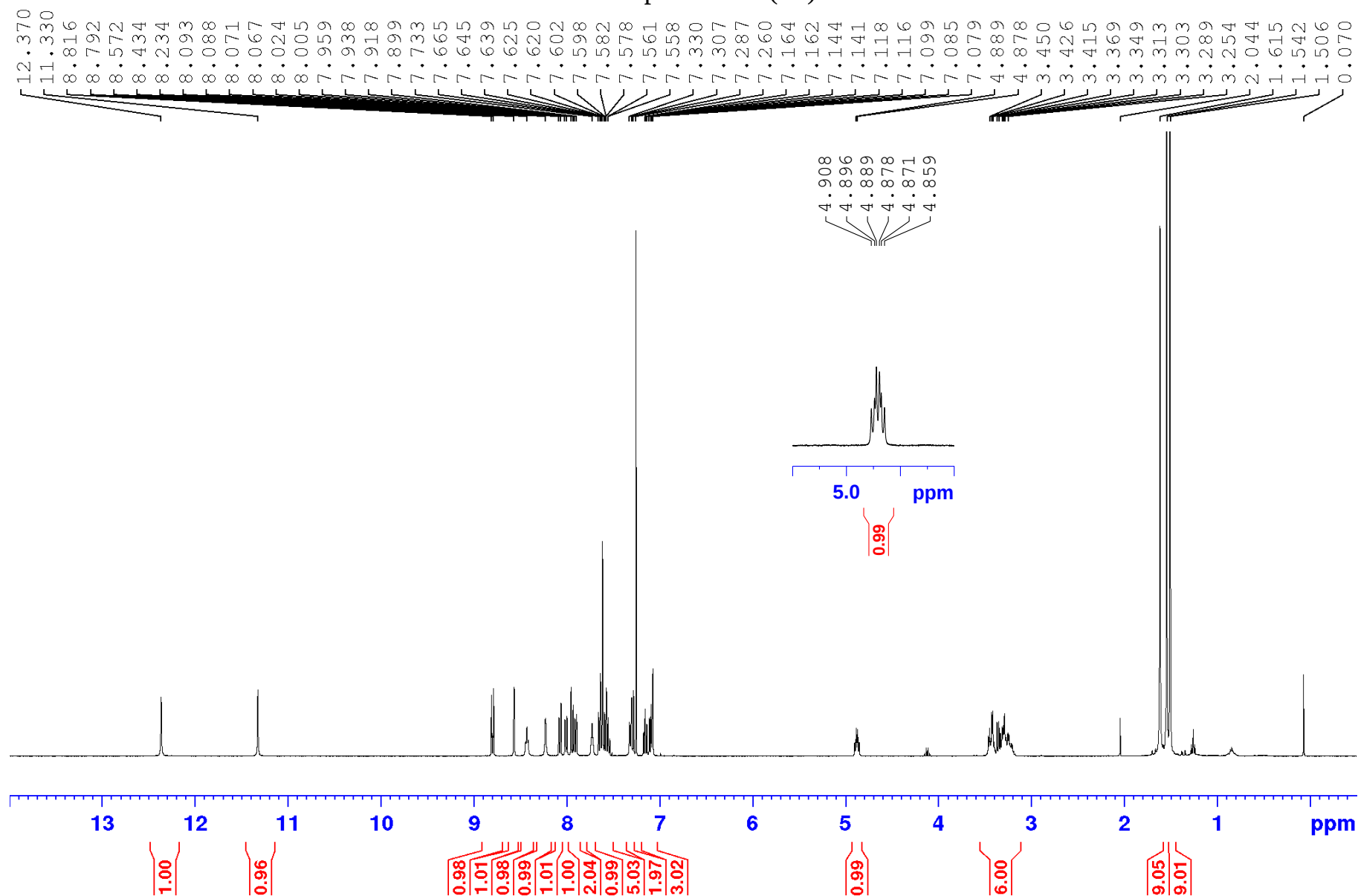


¹H NMR spectra of (S)-N-(4-chloro-2-((1-((2-diBocguanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (6c)

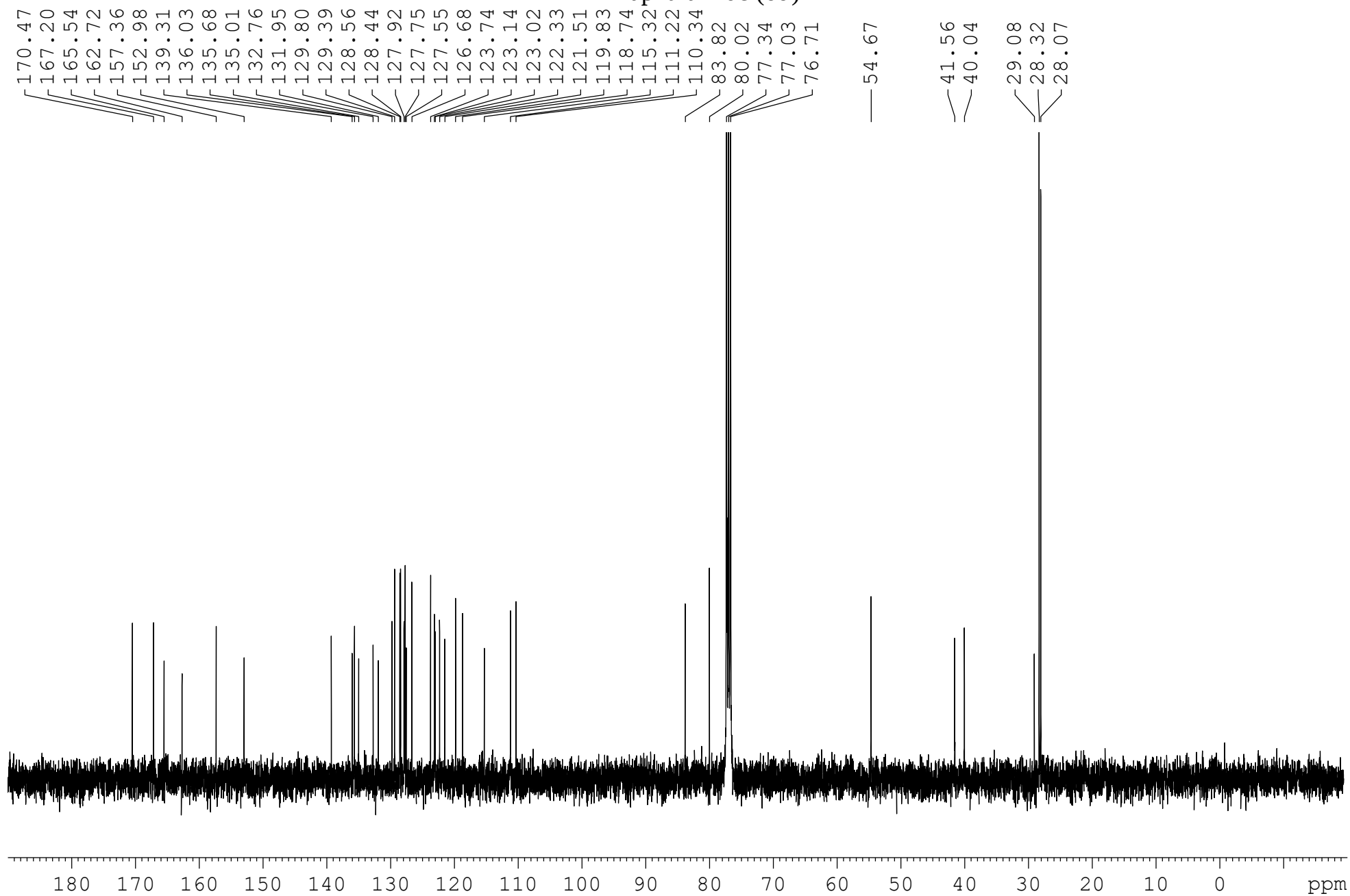


¹³C NMR spectra of (S)-N-(4-chloro-2-((1-((2-diBocguanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**6c**)

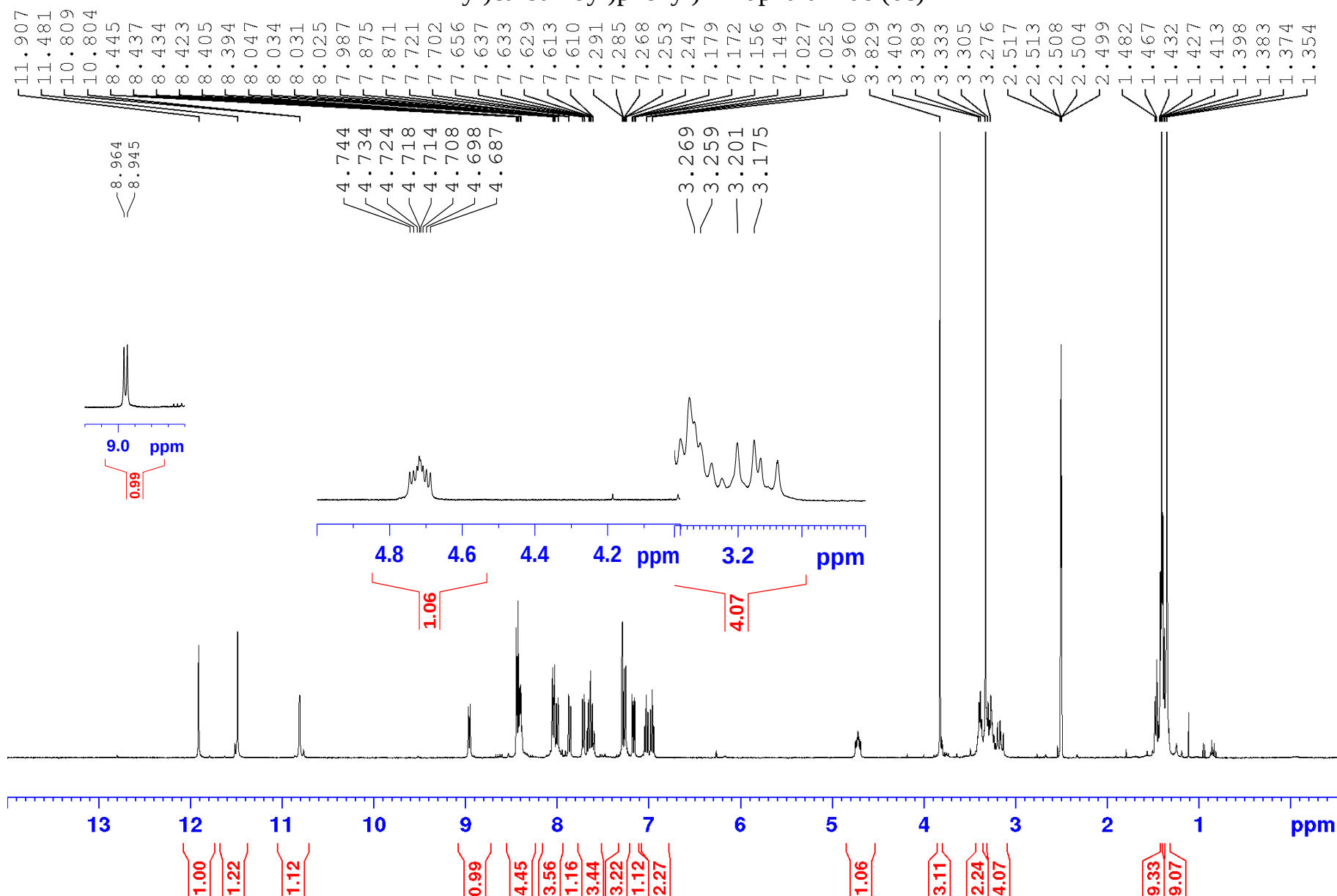


¹H NMR spectra of (S)-N-(4-bromo-2-((1-((2-diBocguanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**6d**)

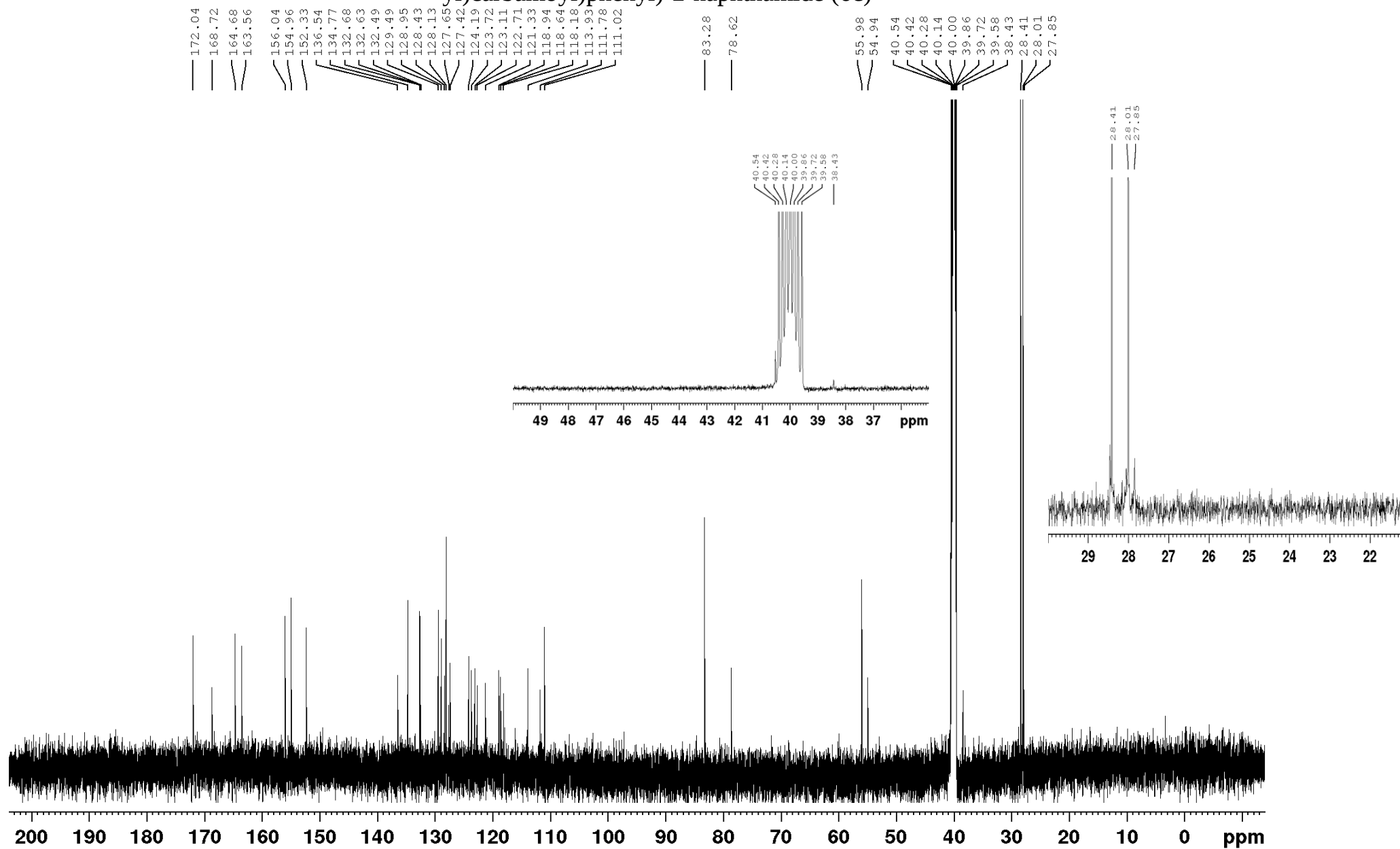
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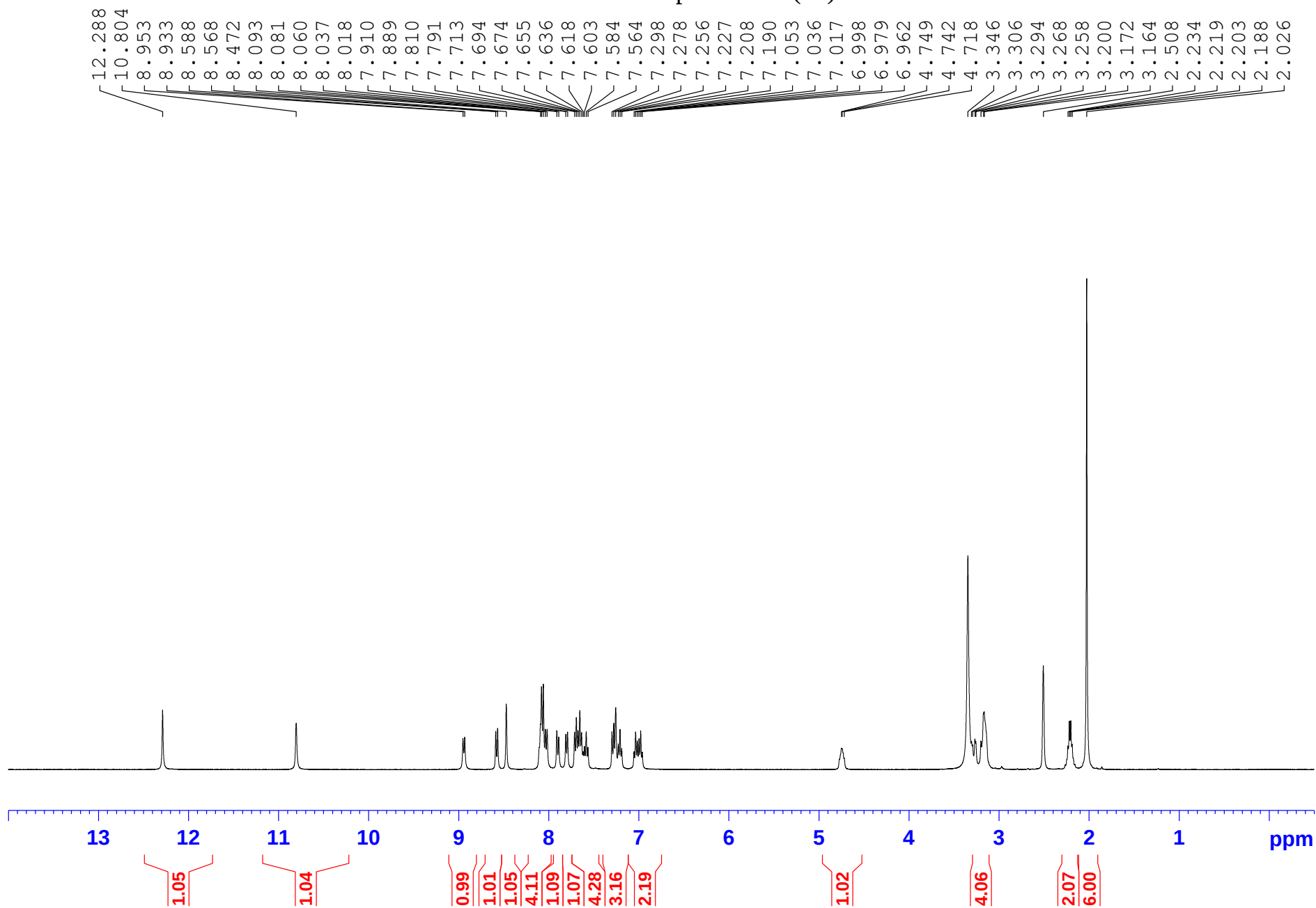
¹H NMR spectra of (S)-N-(4-methoxy-2-((1-((2-diBocguanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**6e**)



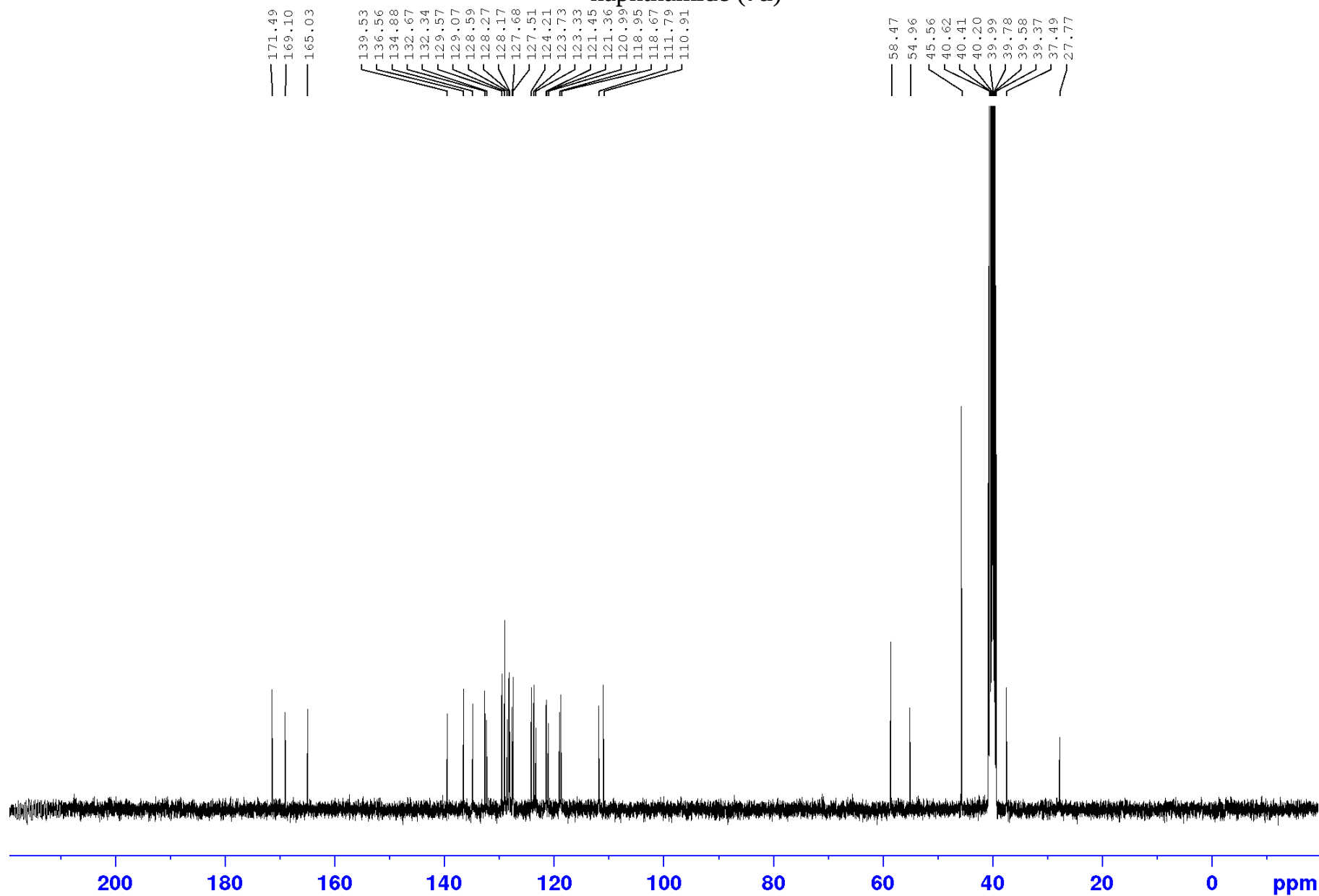
^{13}C NMR spectra of (*S*)-*N*-(4-methoxy-2-((1-((2-diBocguanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**6e**)



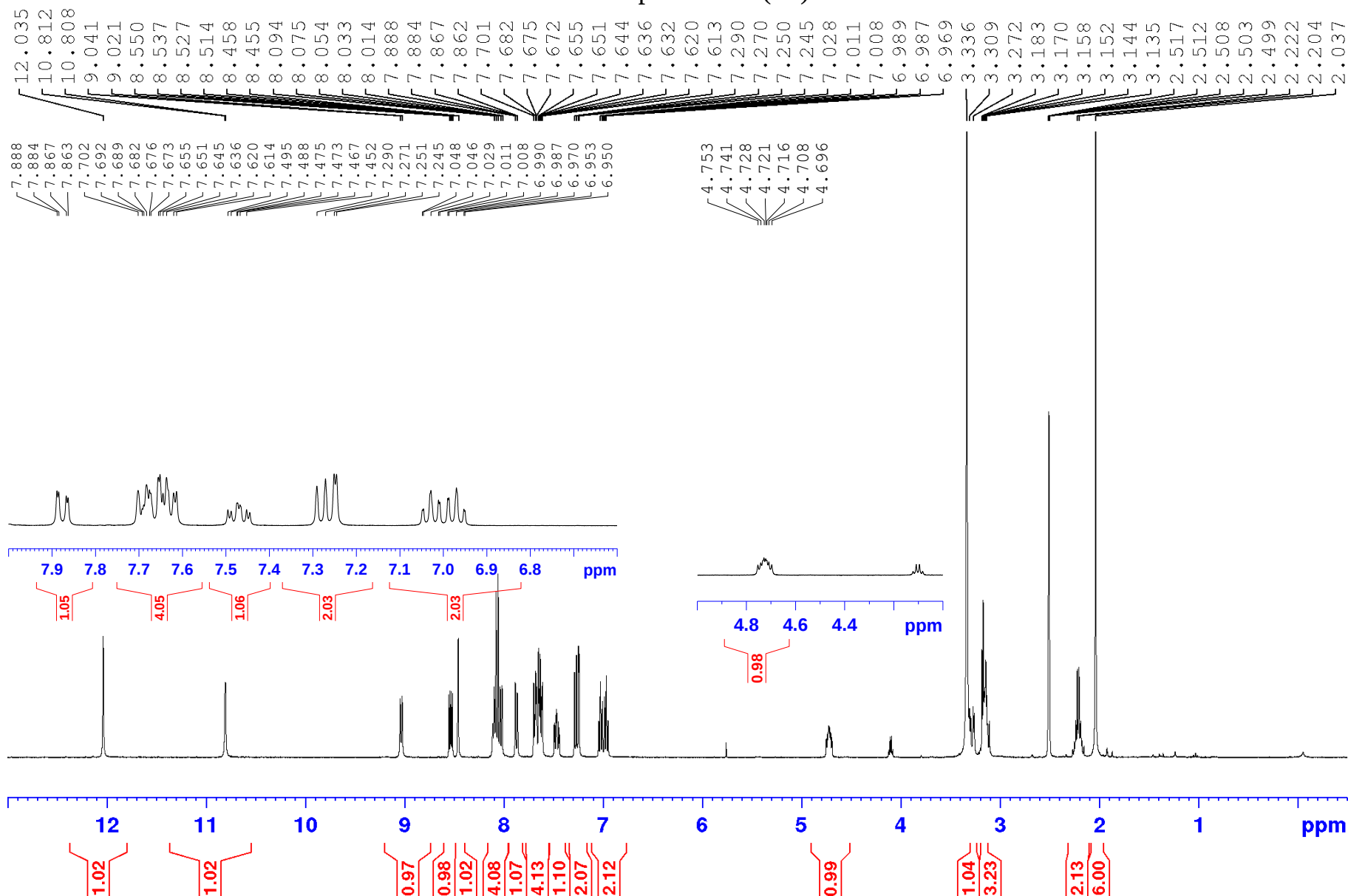
¹H NMR spectra of (S)-N-(2-((1-((2-(dimethylamino)ethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (7a)



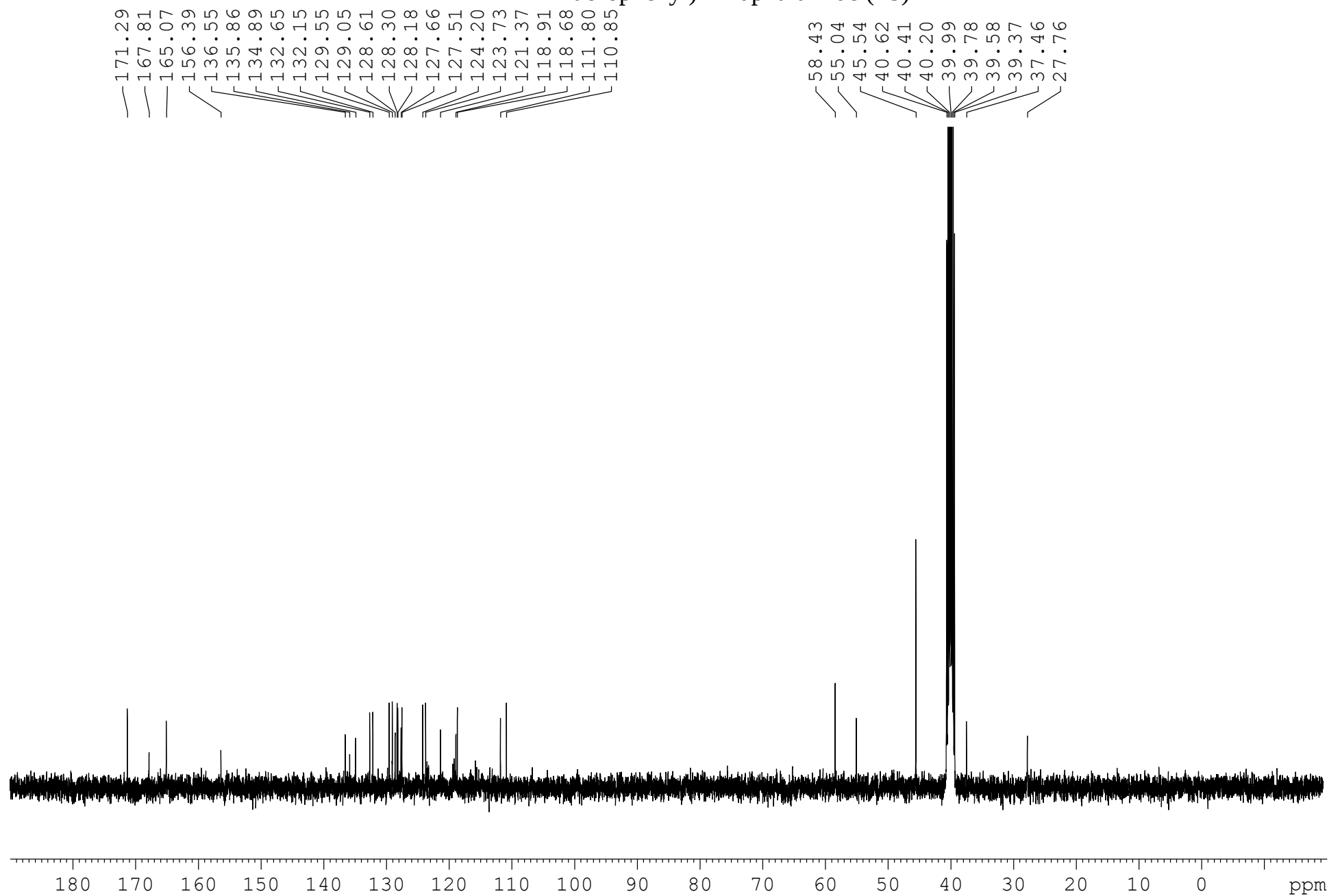
^{13}C NMR spectra of (S)-N-(2-((1-((2-(dimethylamino)ethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (7a)



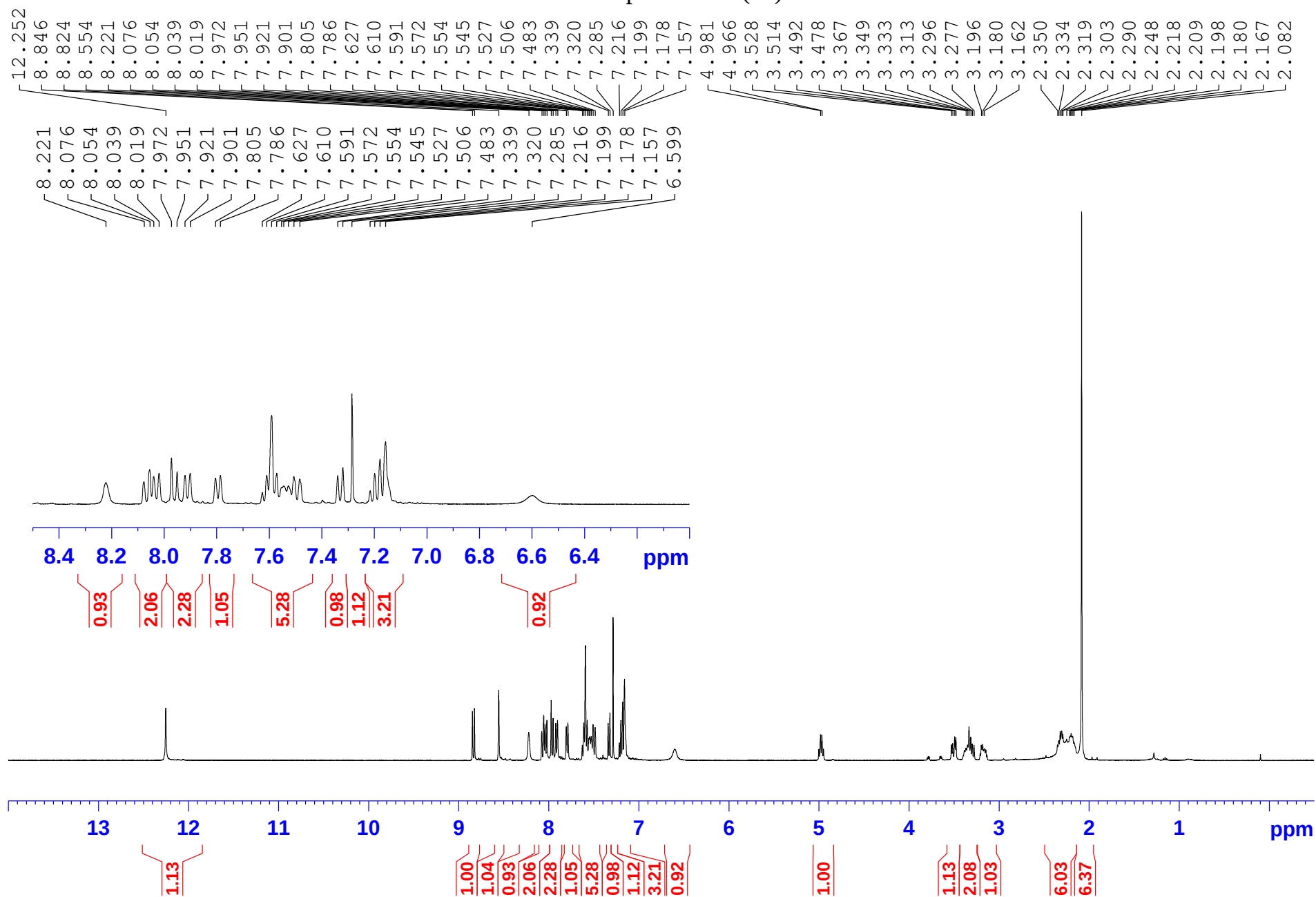
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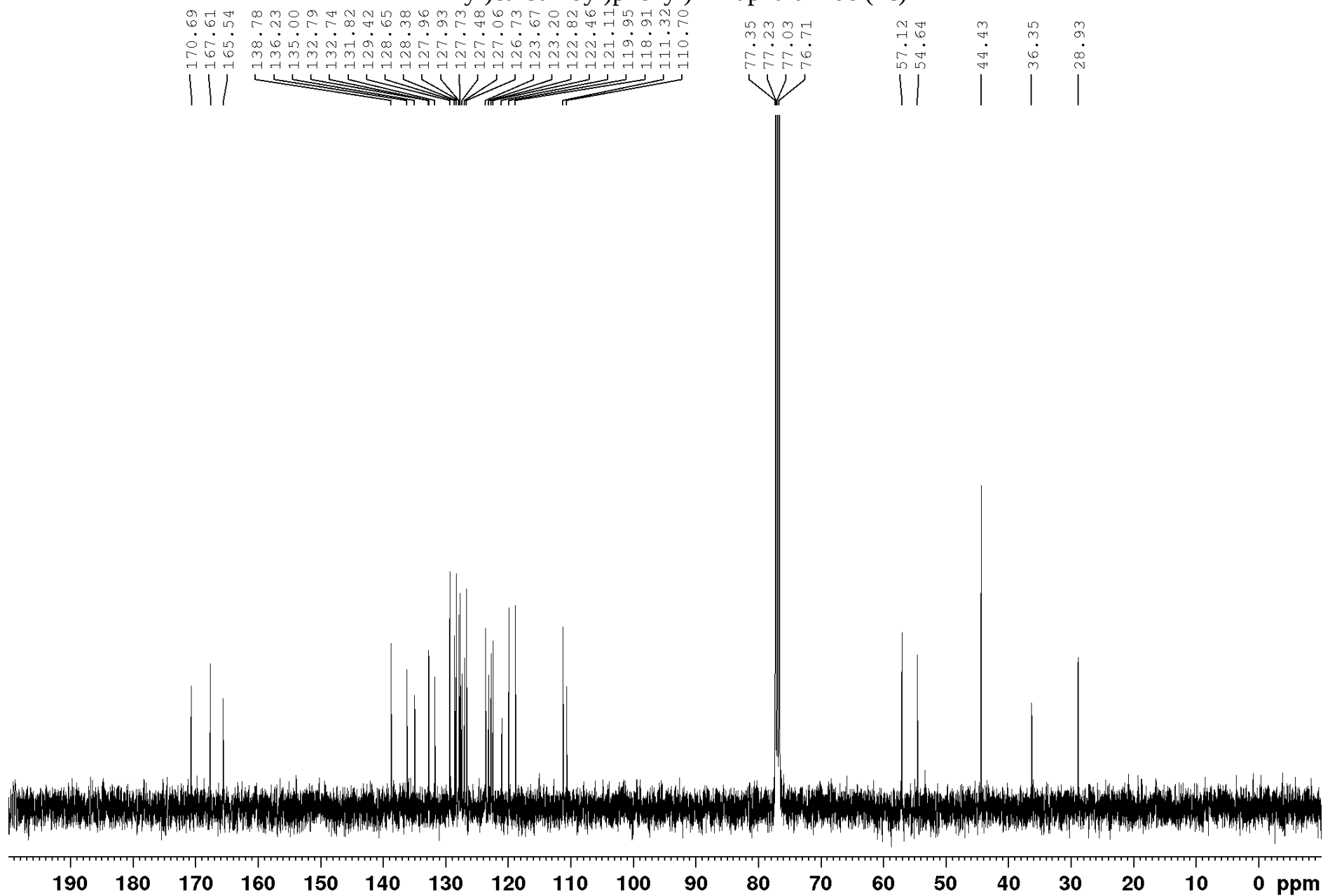
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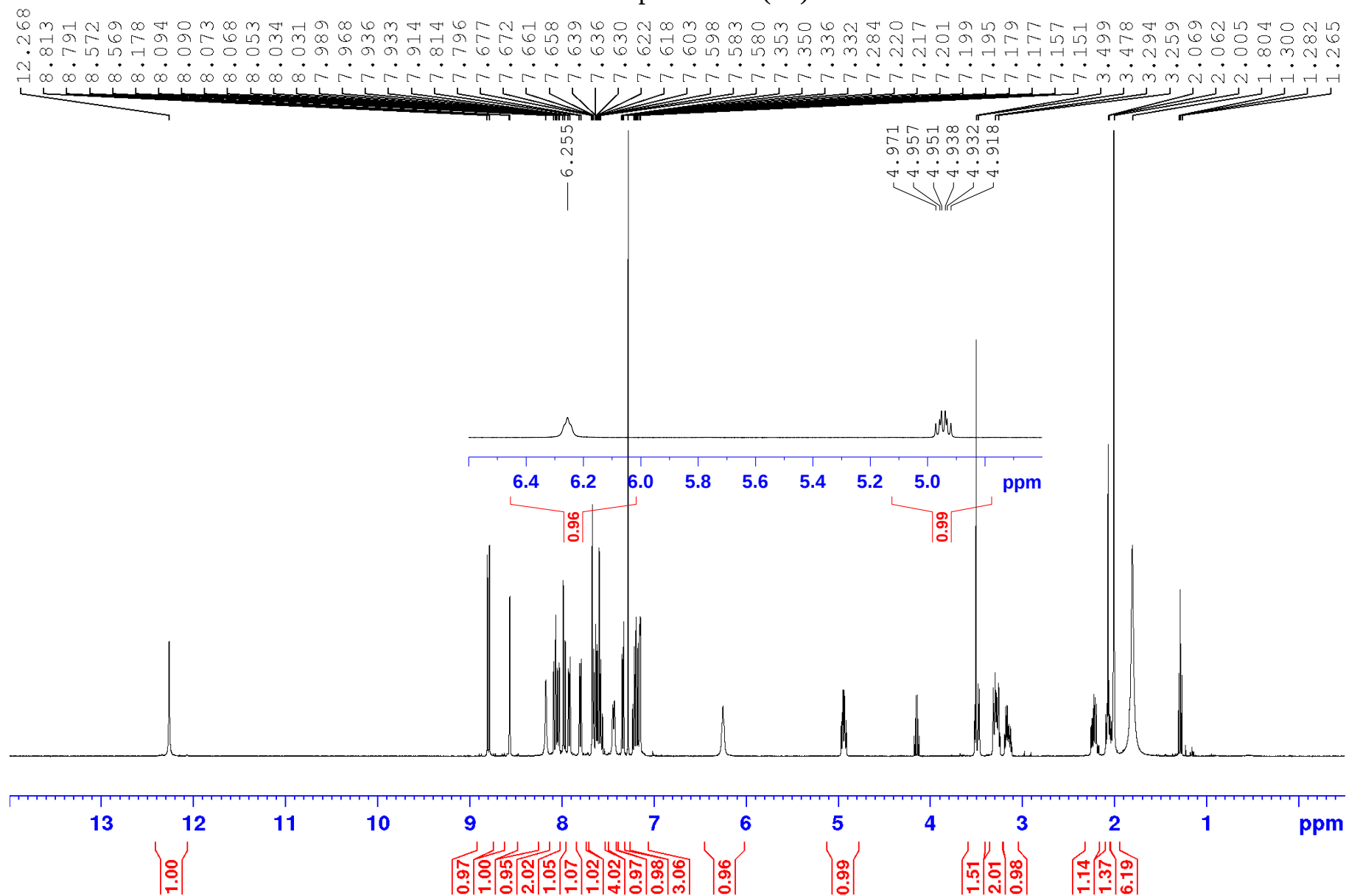
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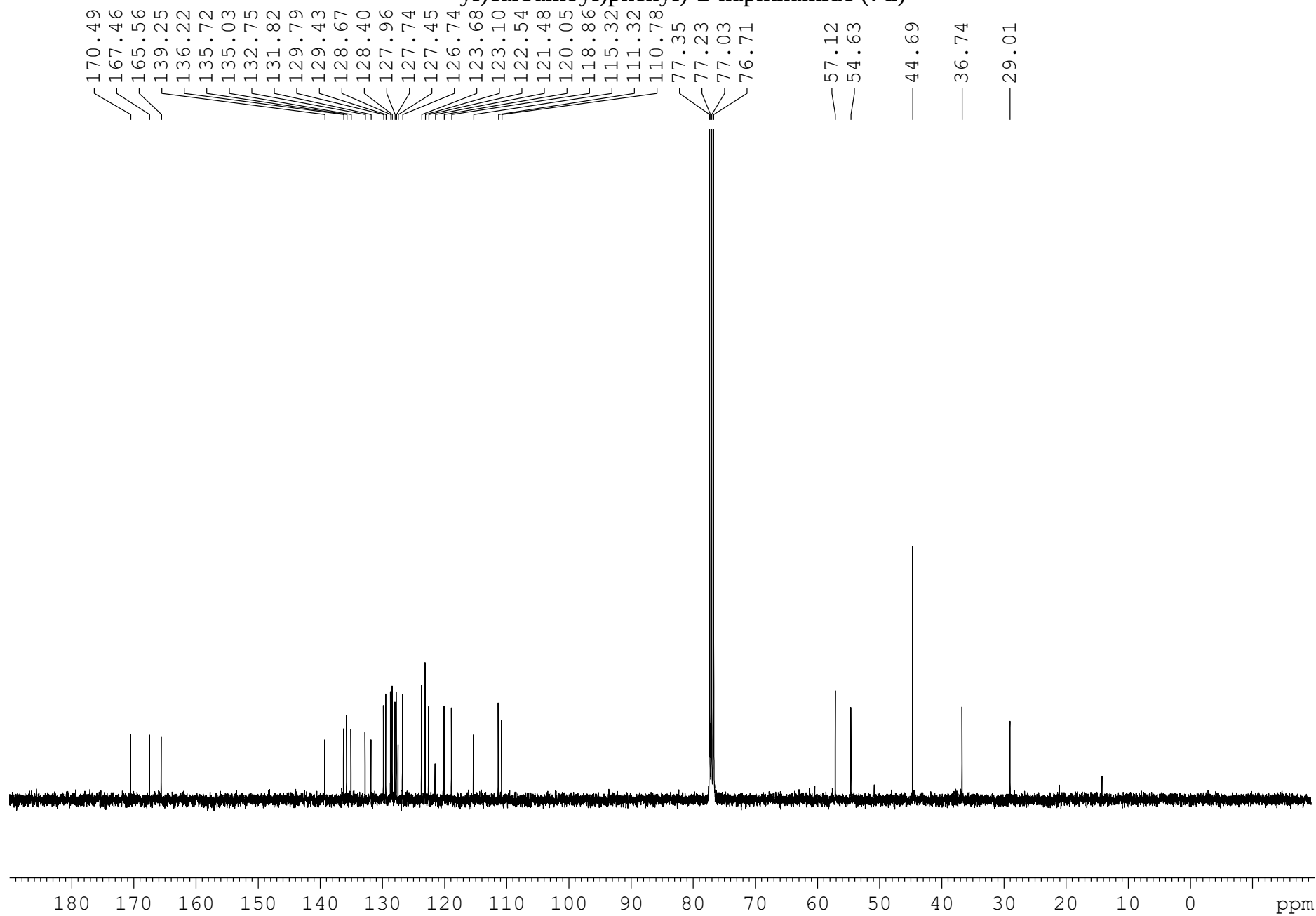
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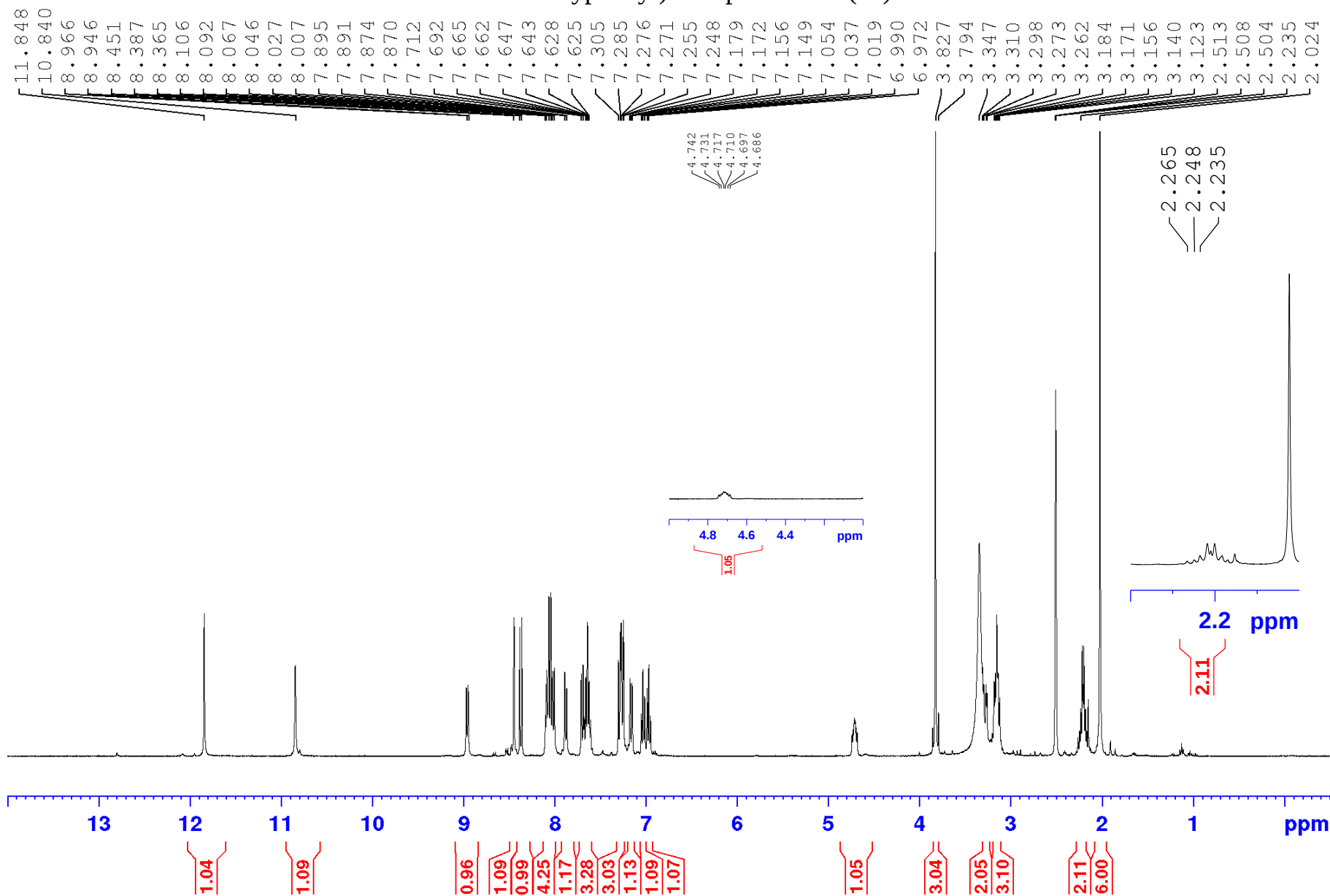
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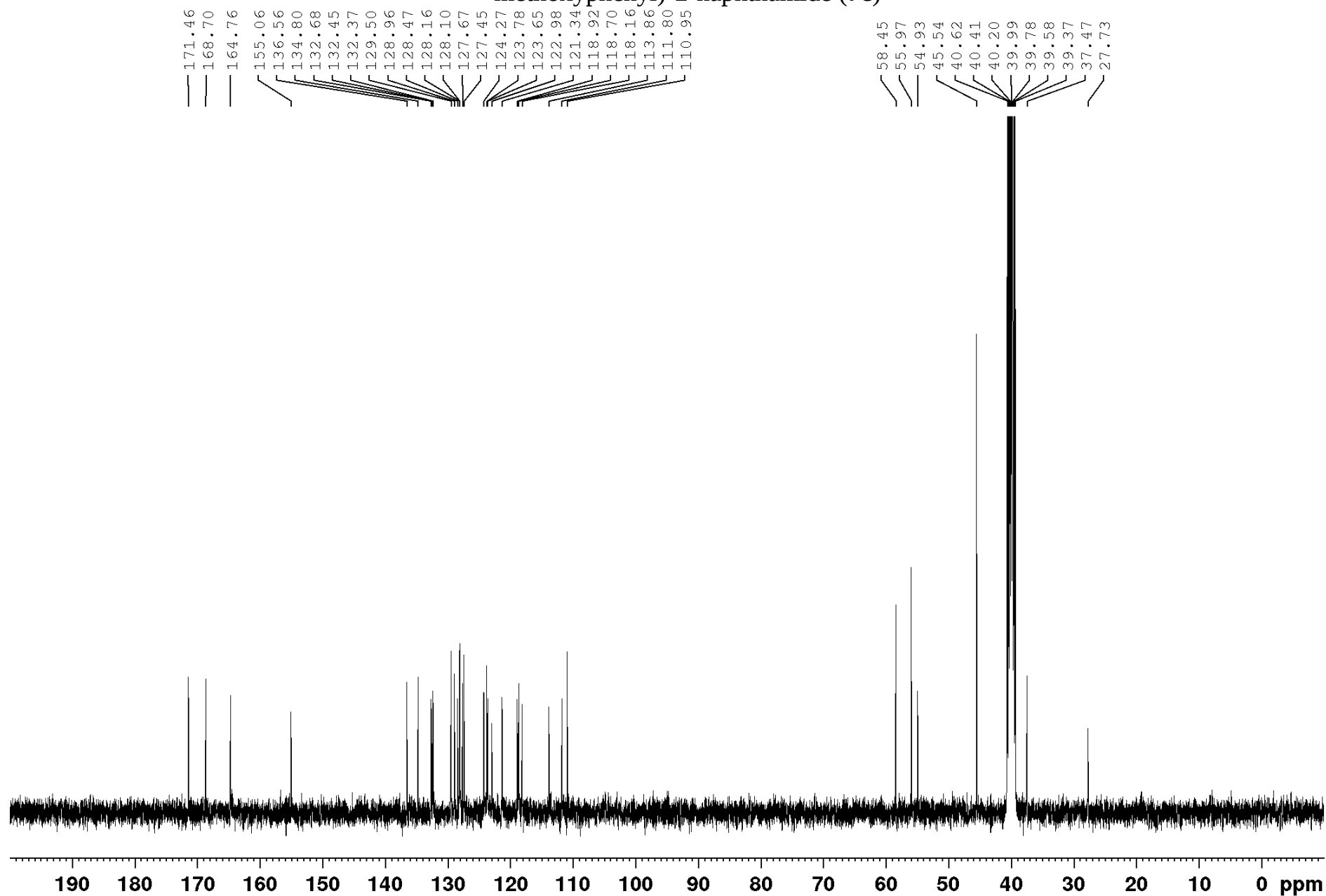
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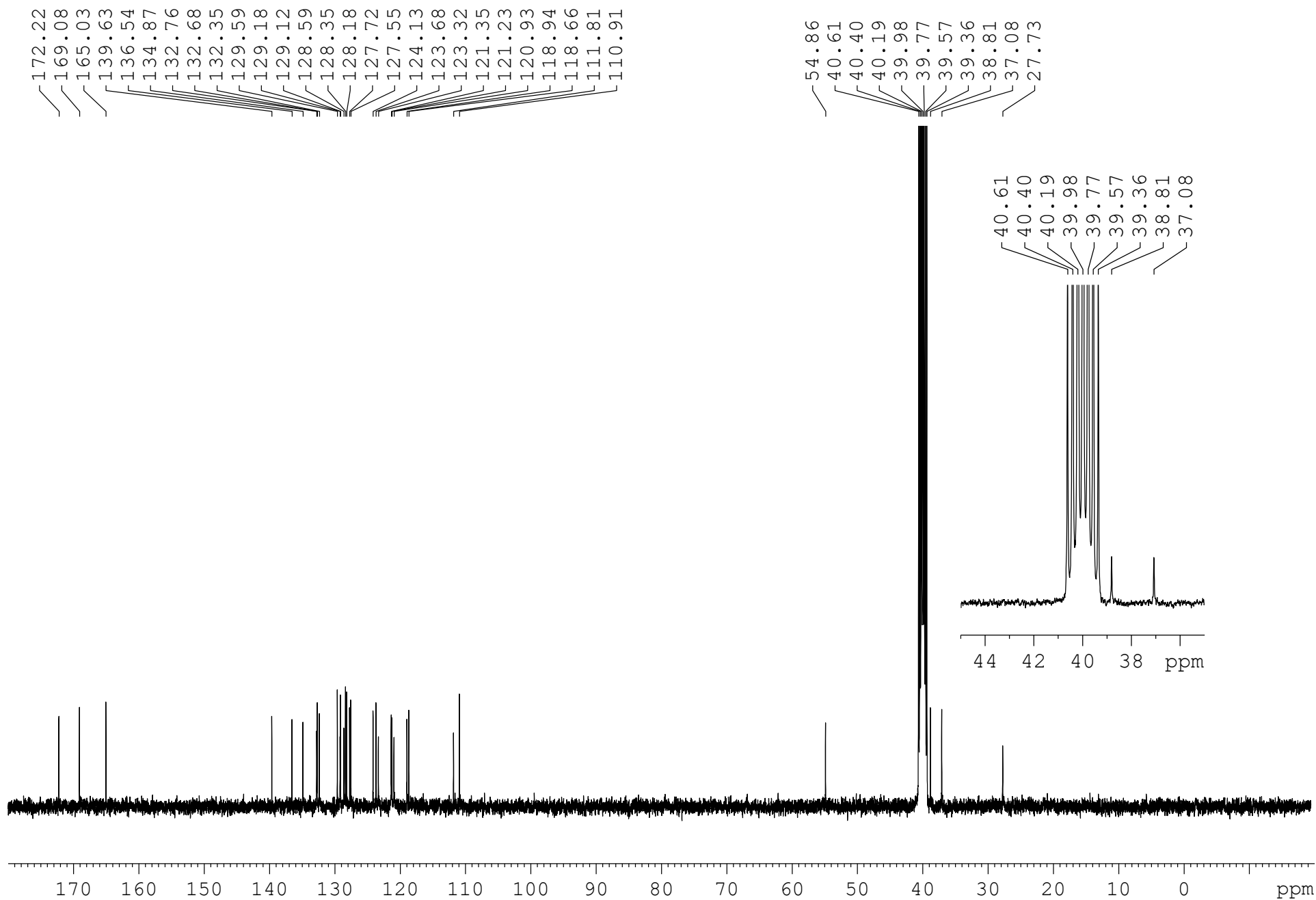
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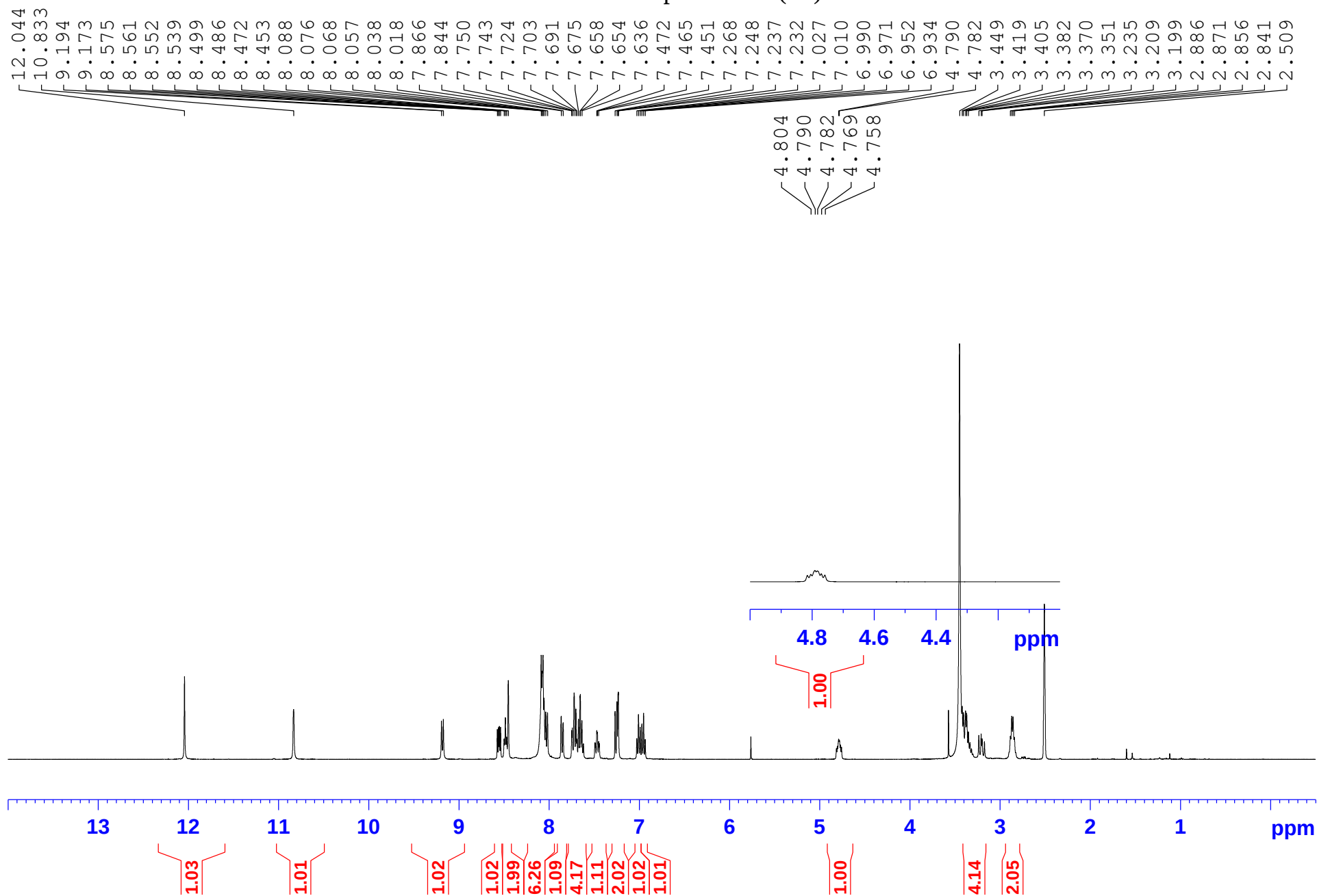
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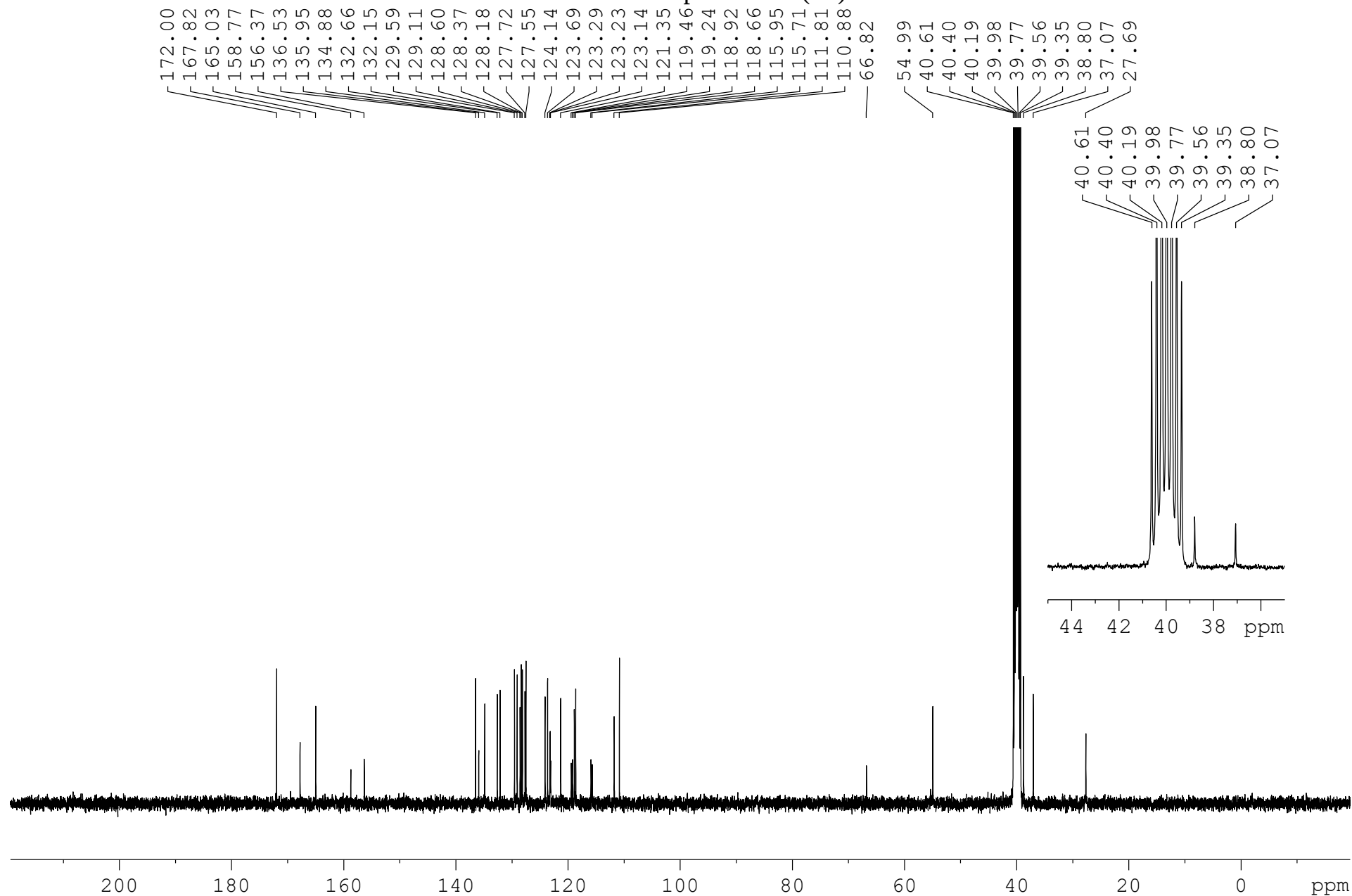
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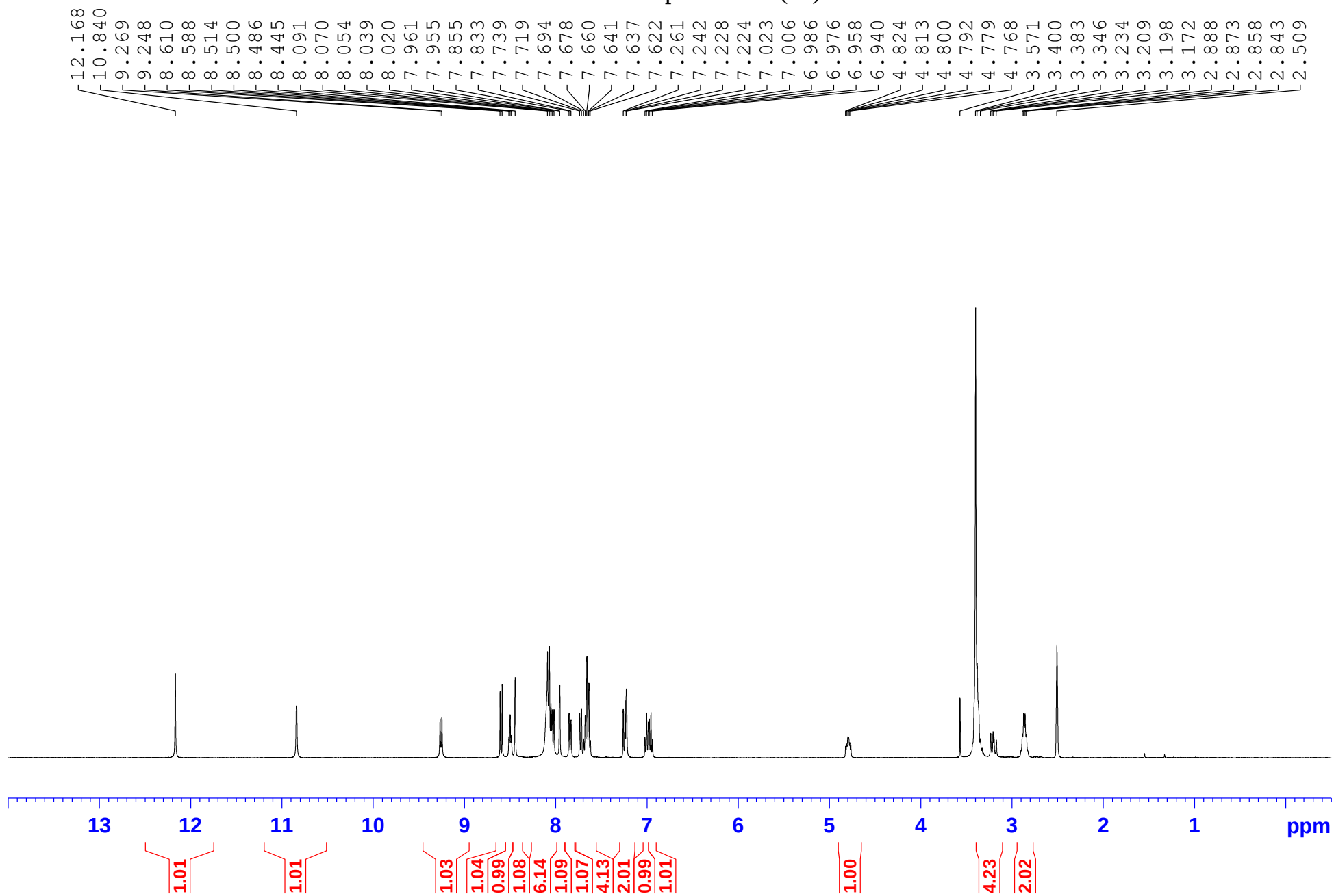
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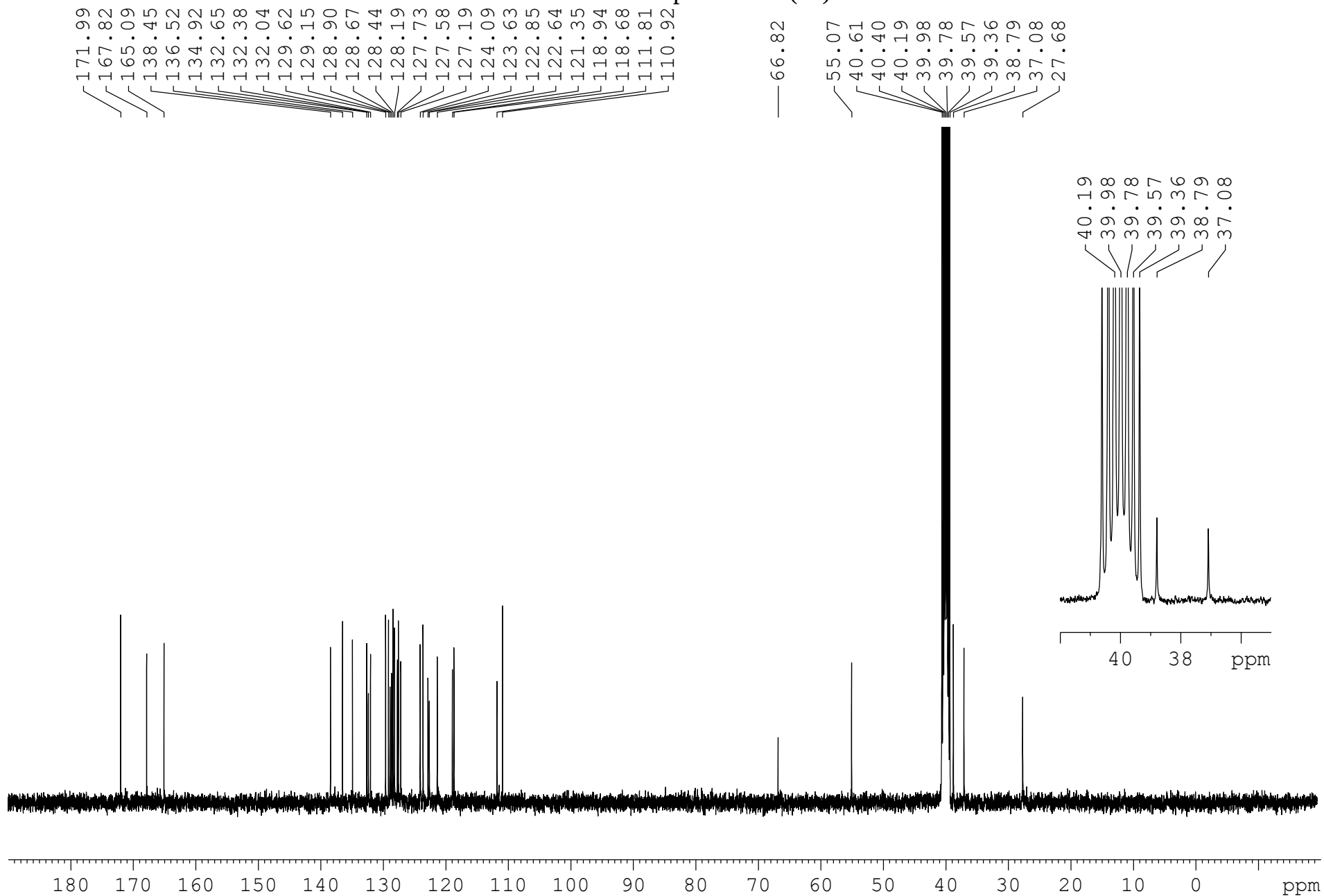
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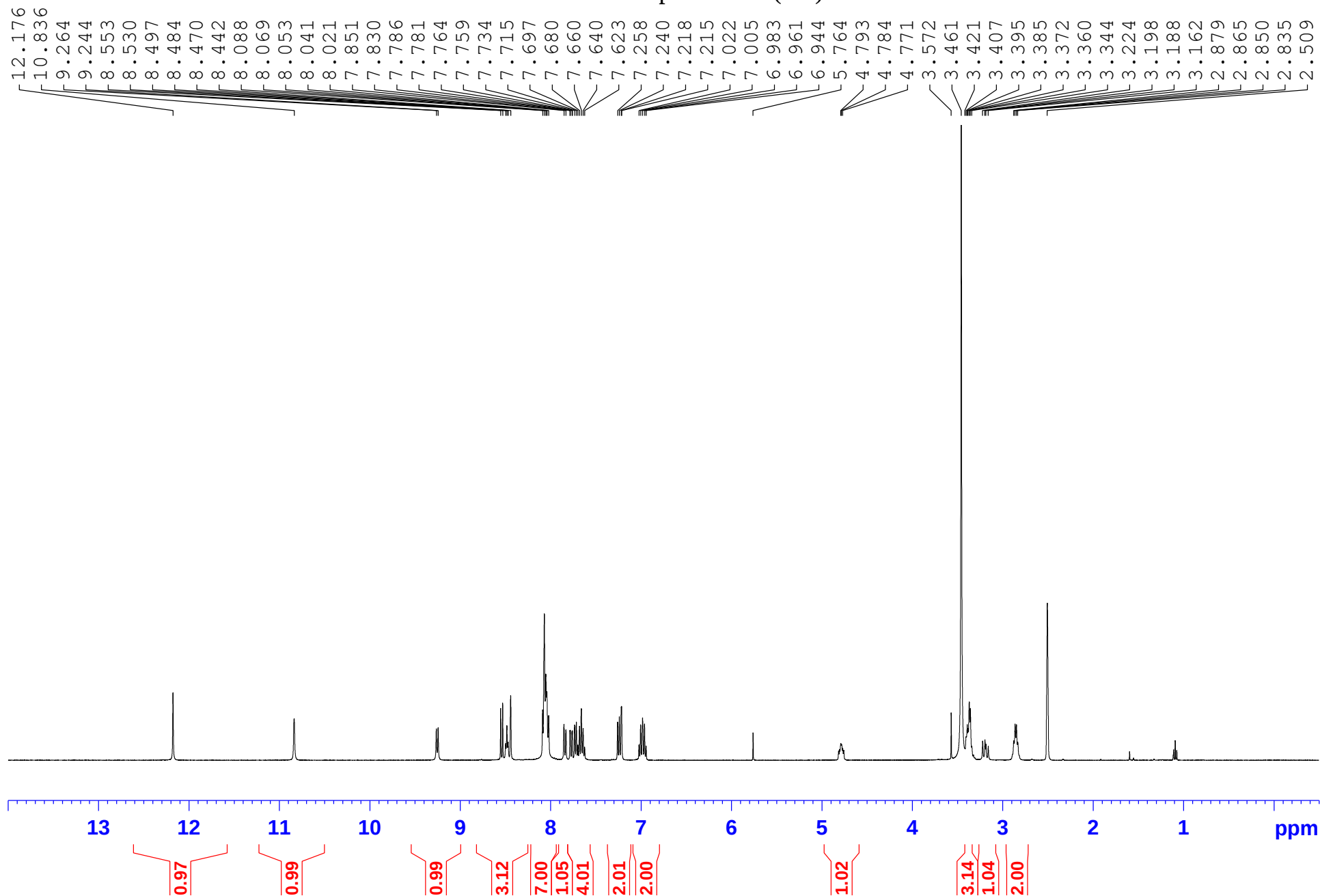
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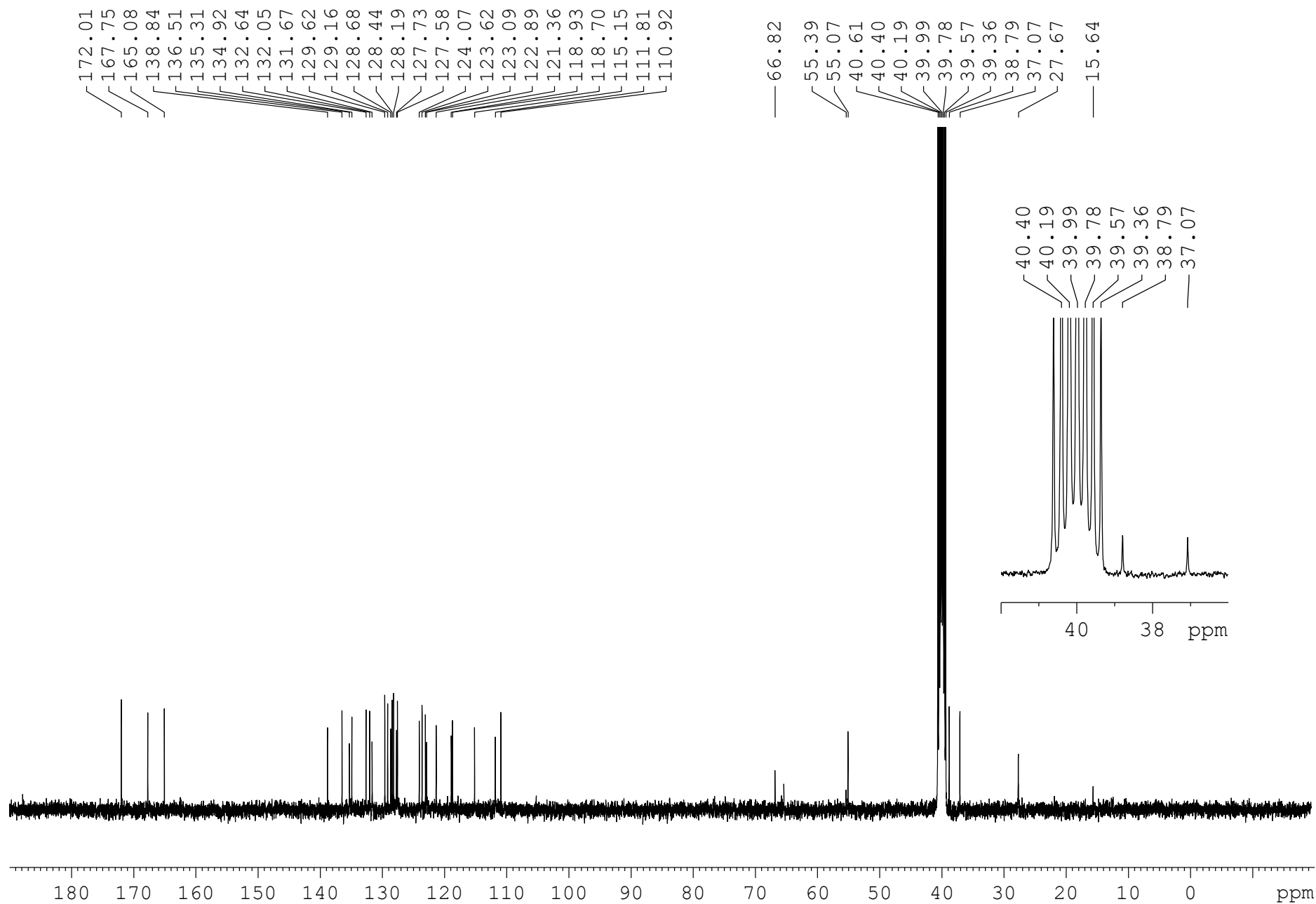
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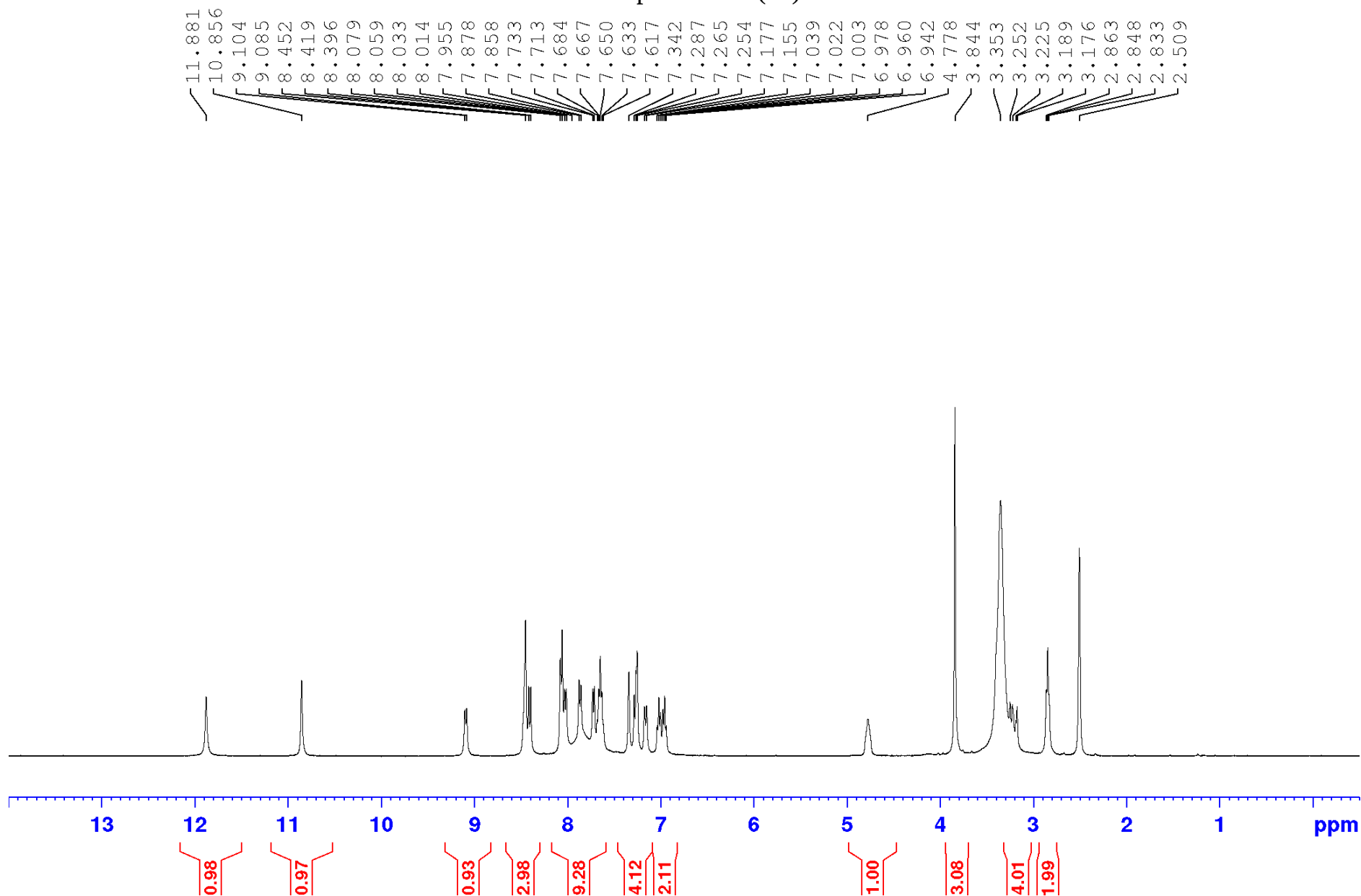
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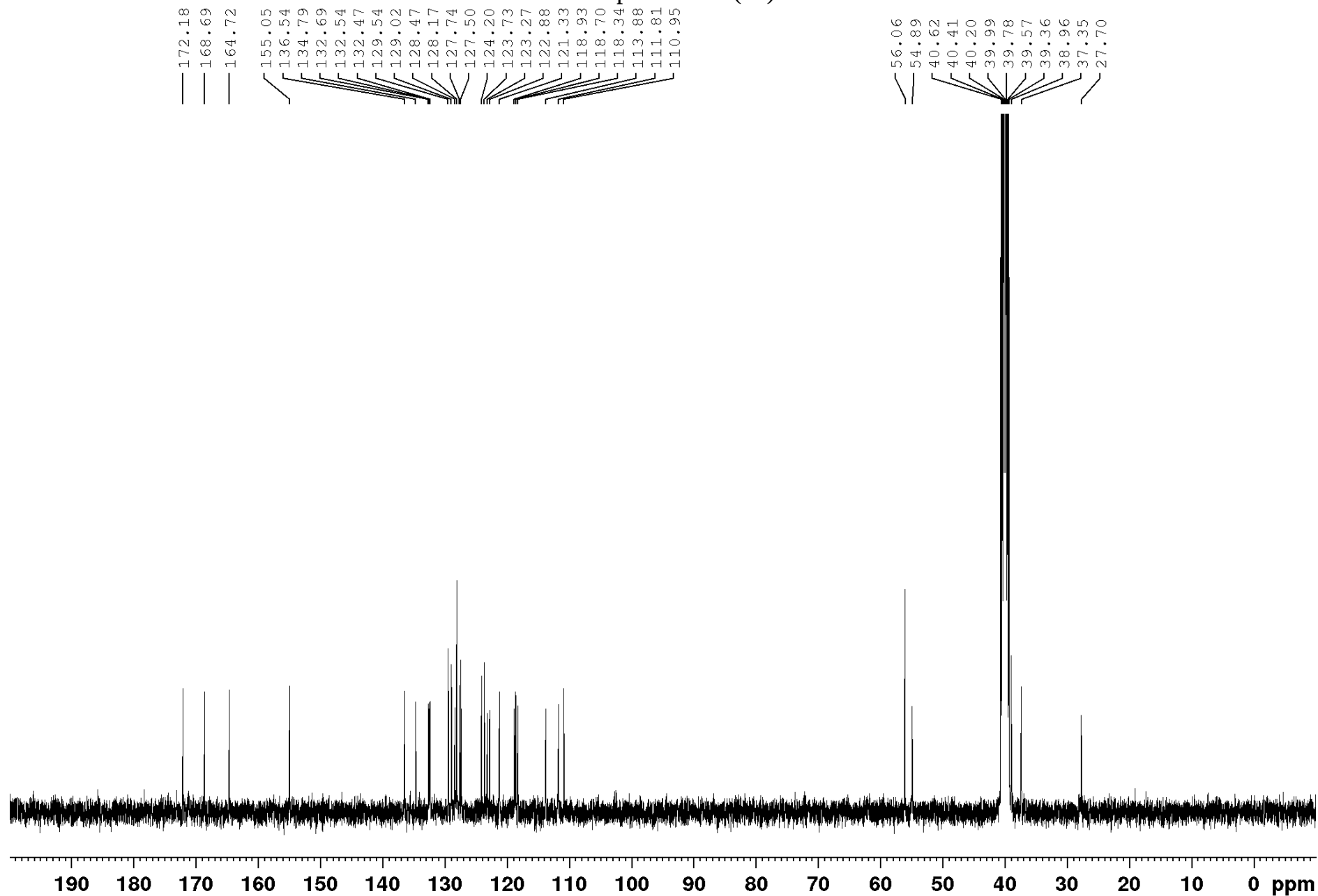
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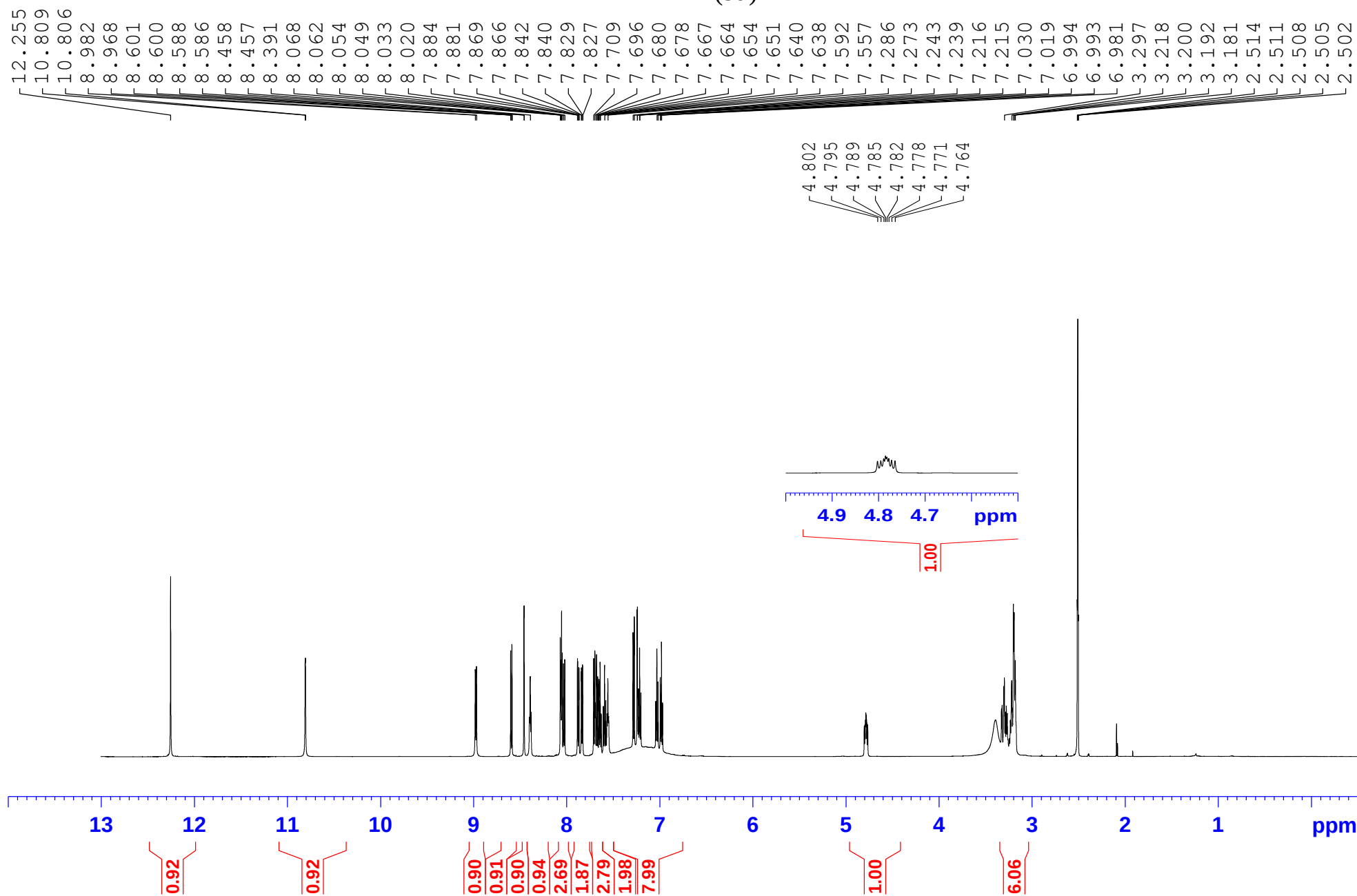
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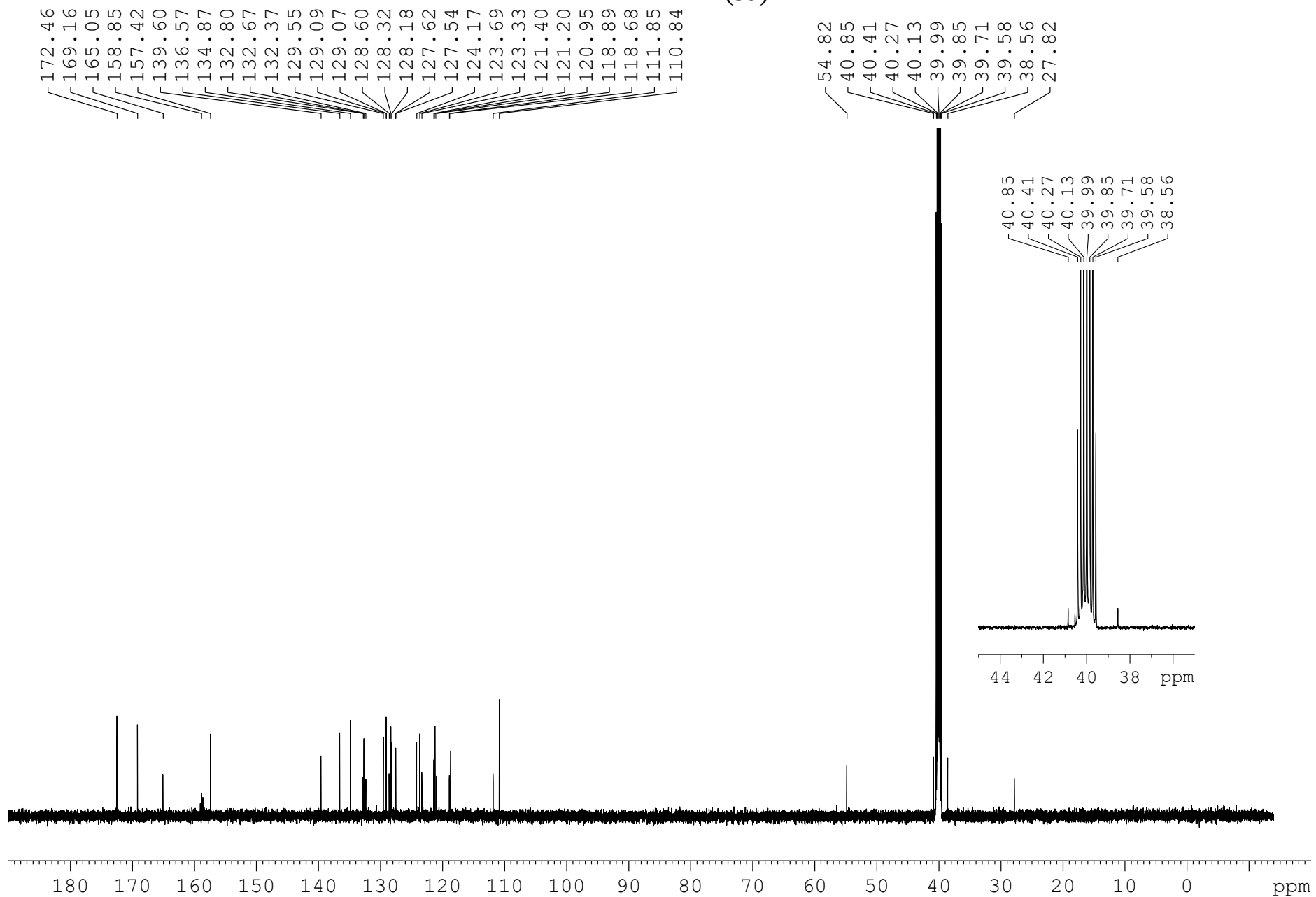
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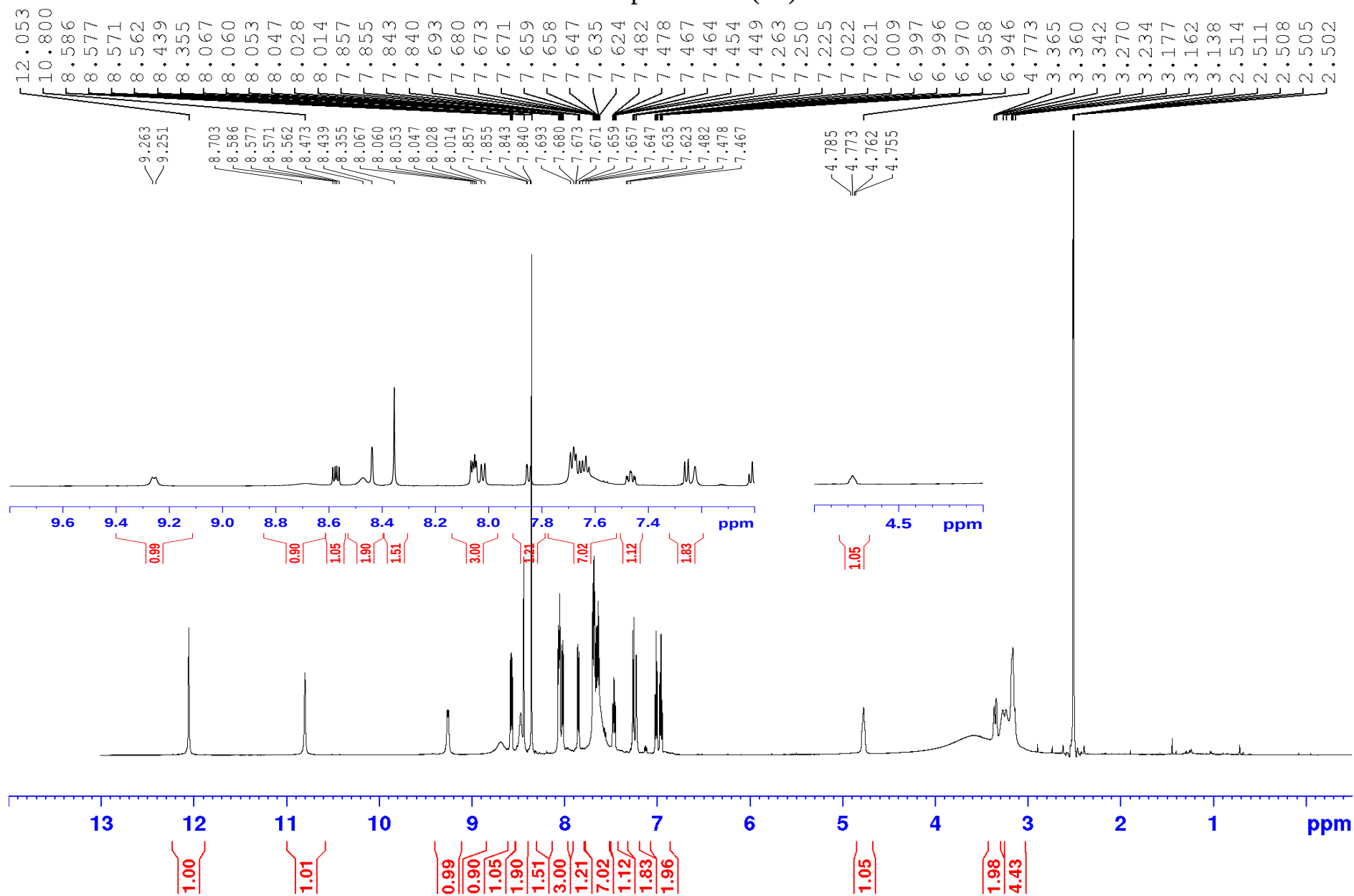
¹H NMR spectra of (S)-N-(2-((1-((2-guanidinoethyl)amino)-3-(1H-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide
(9a)



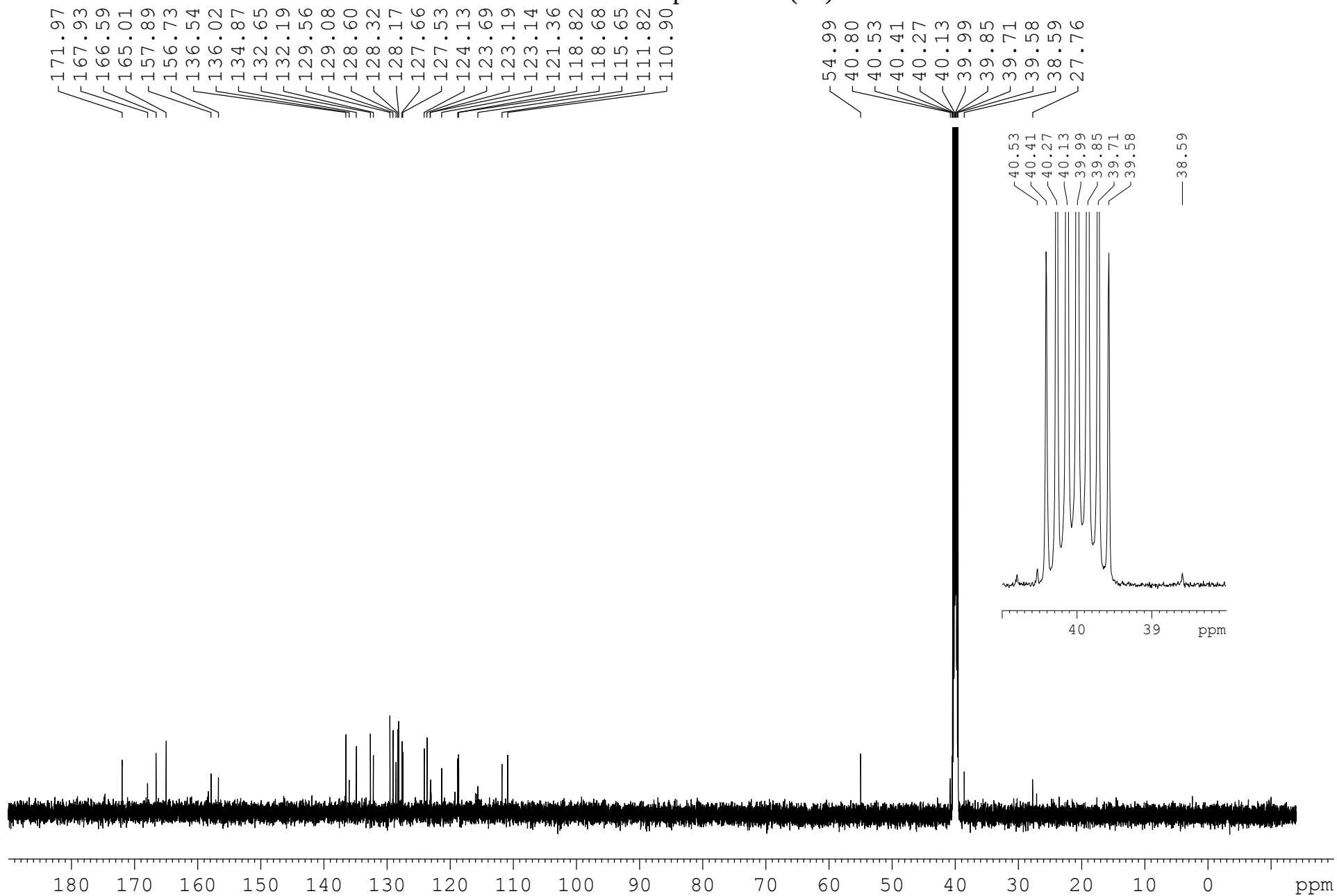
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(9a)



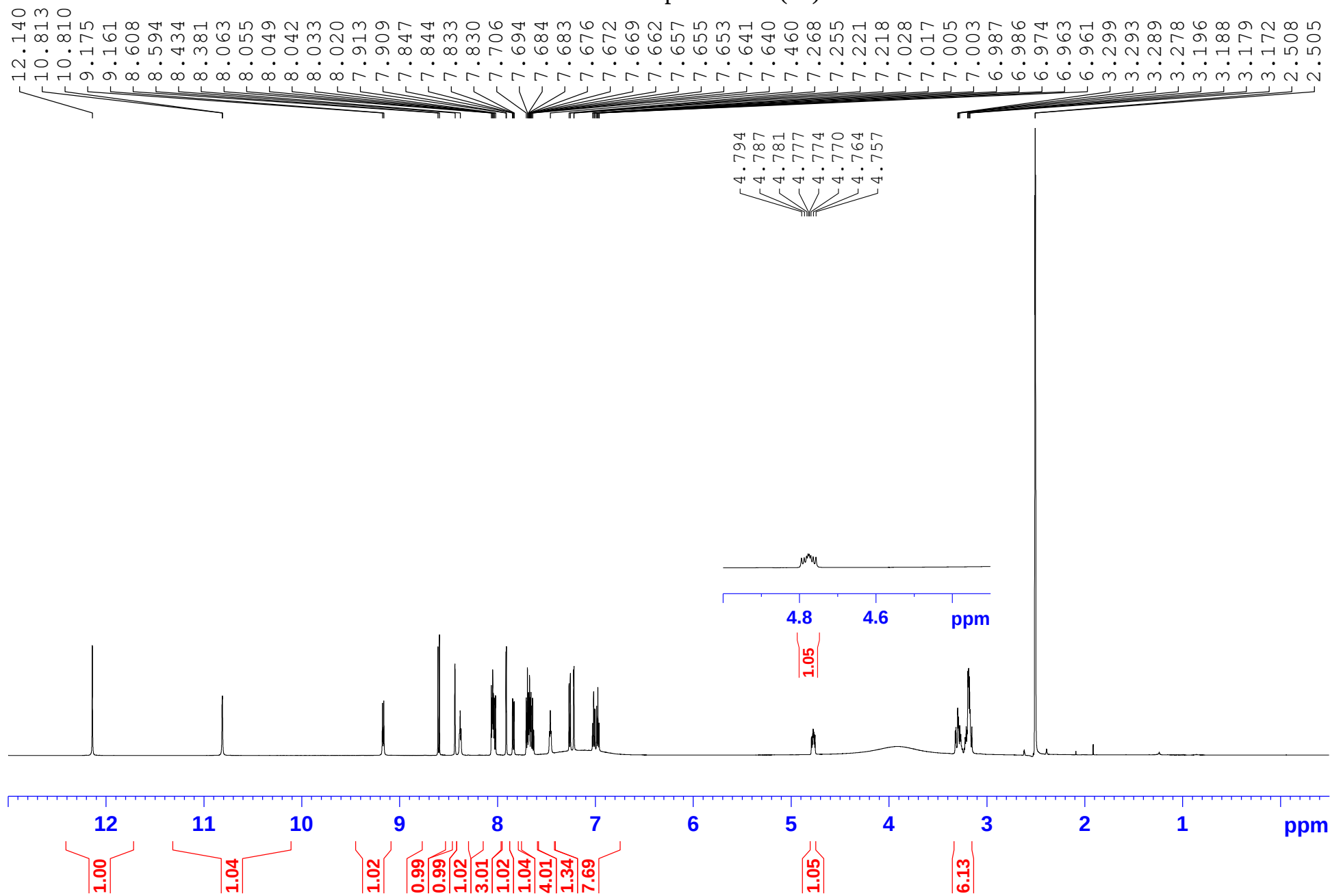
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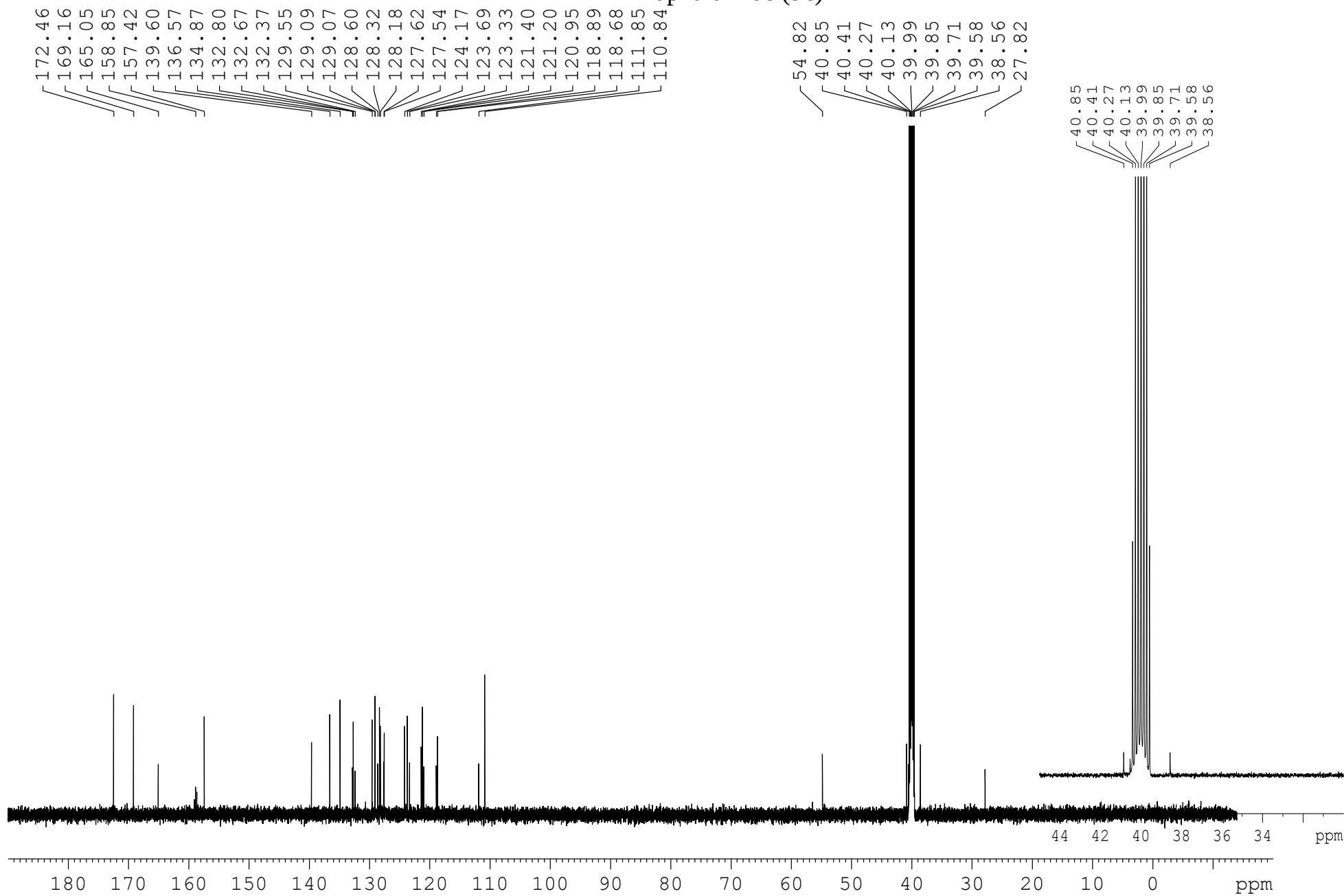
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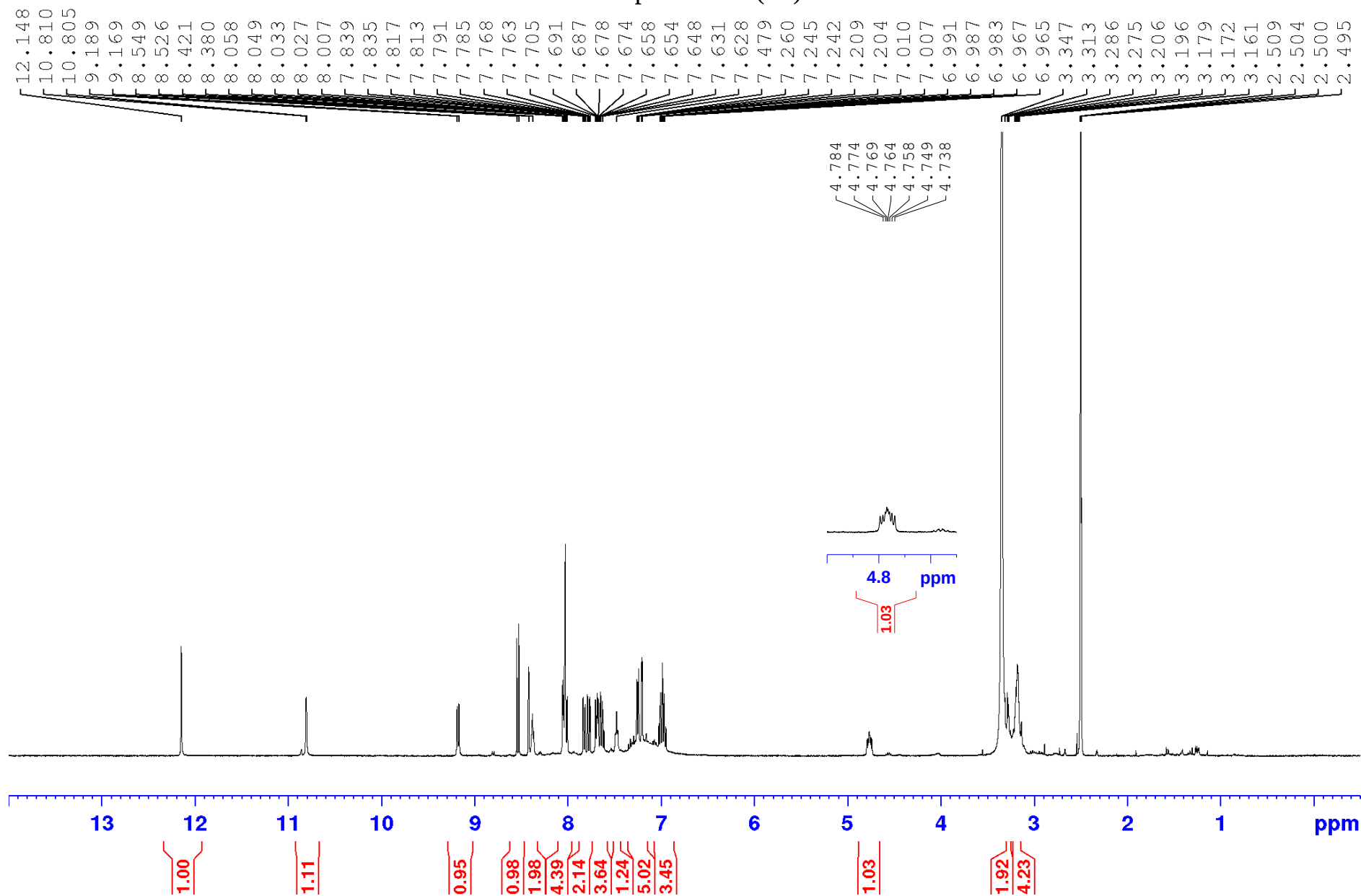
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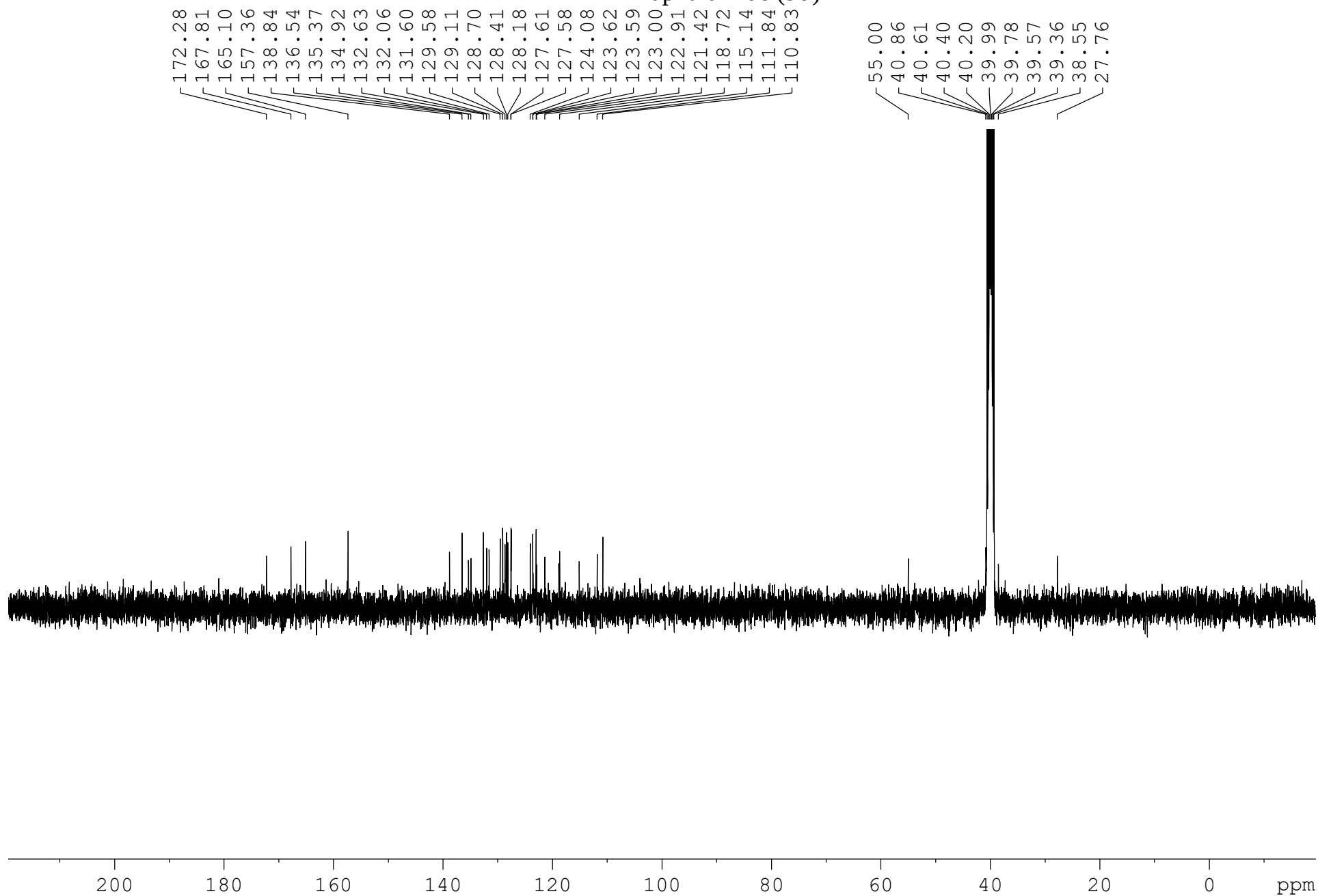
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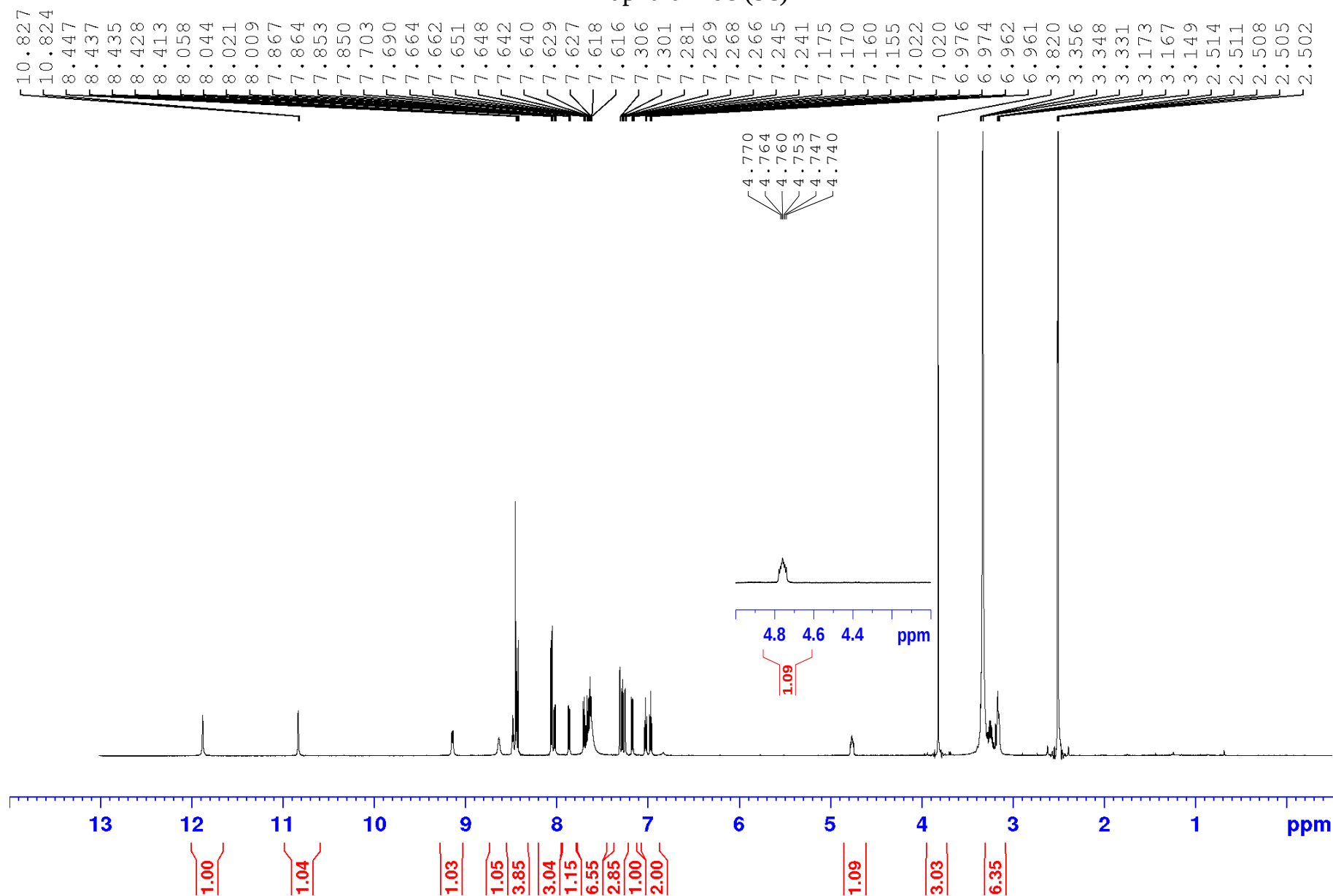
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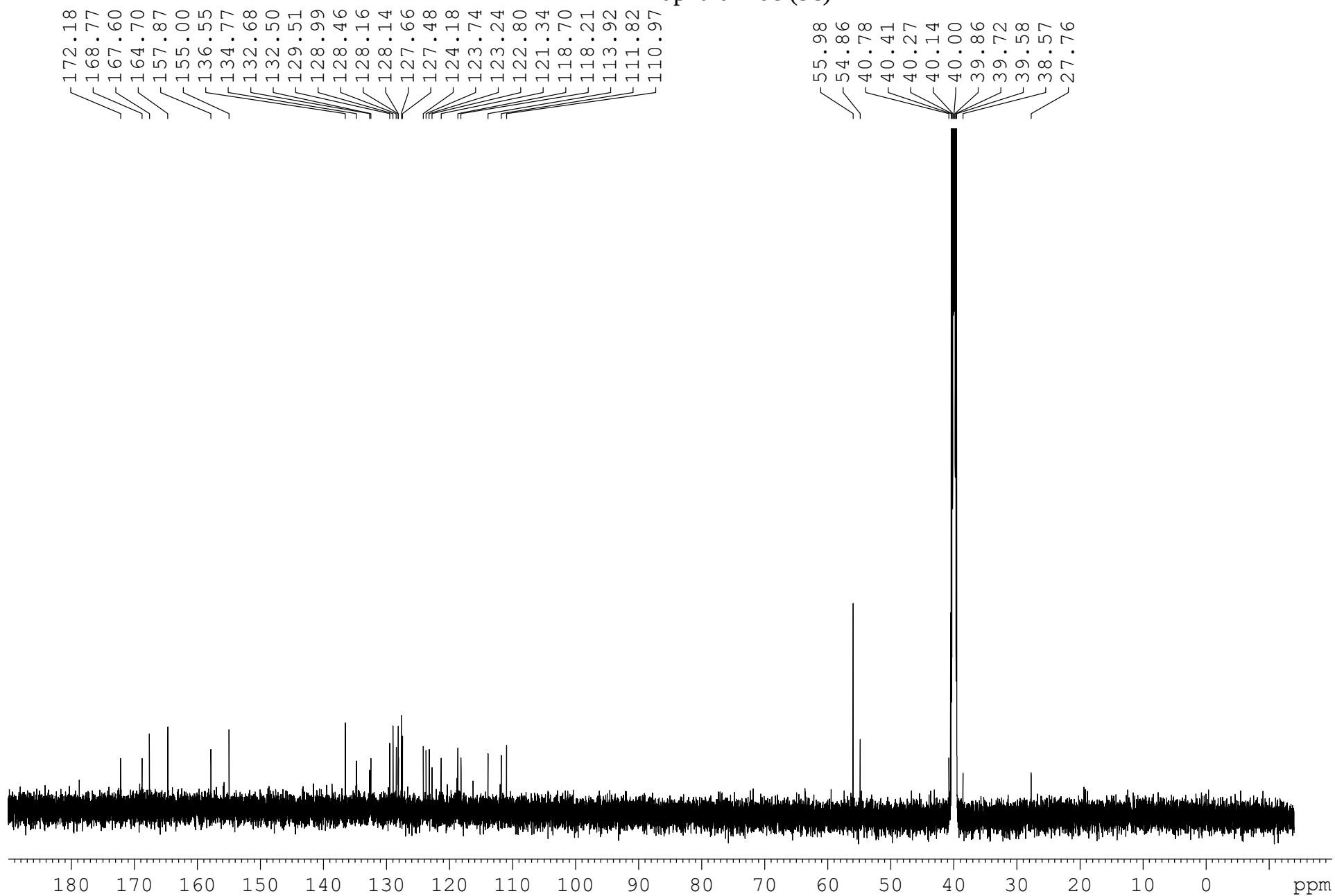
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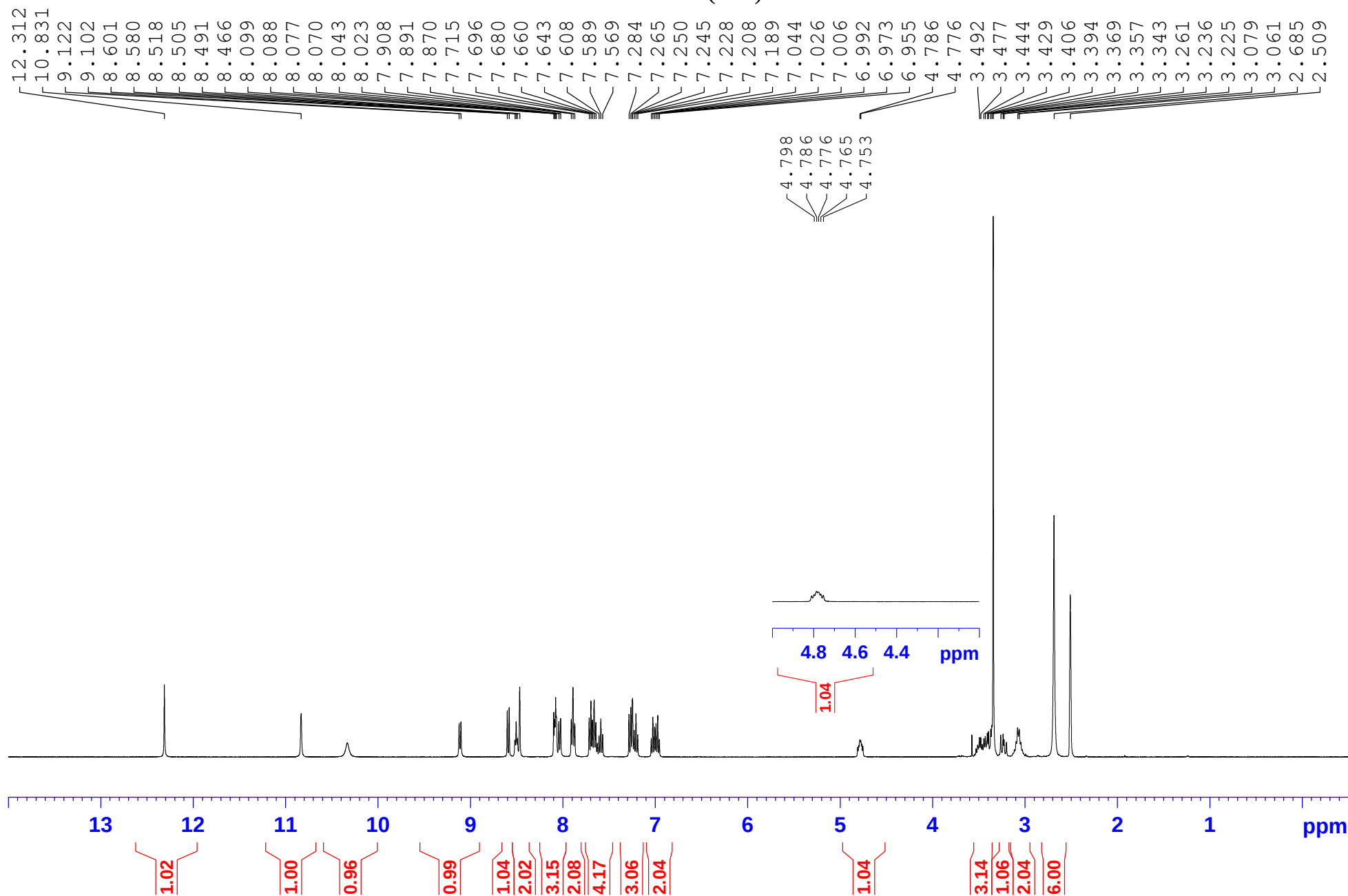
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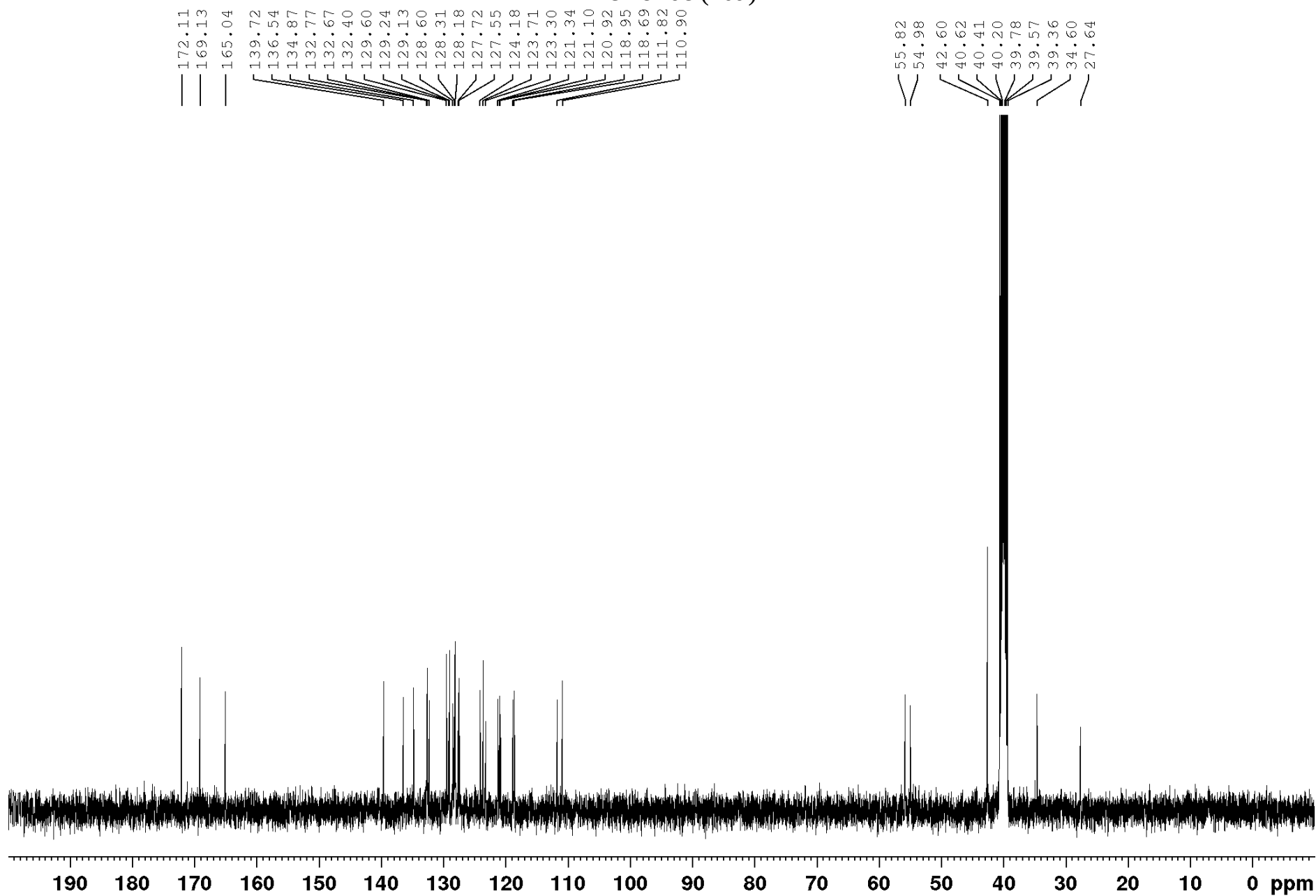
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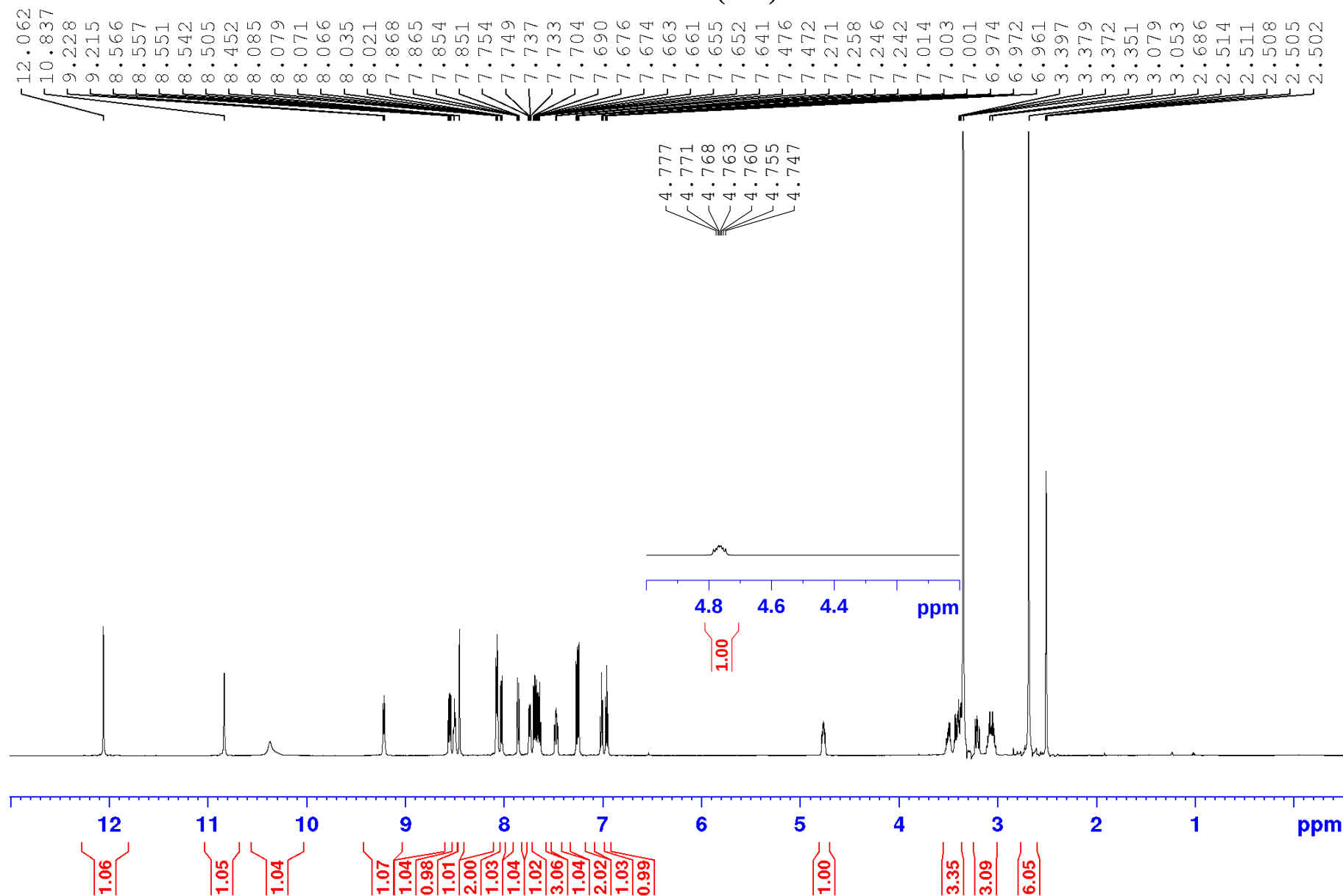
¹H NMR spectra of (S)-2-(2-(2-(2-naphthamido)benzamido)-3-(1*H*-indol-3-yl)propanamido)-N,N-dimethylethan-1-aminium chloride
(10a)



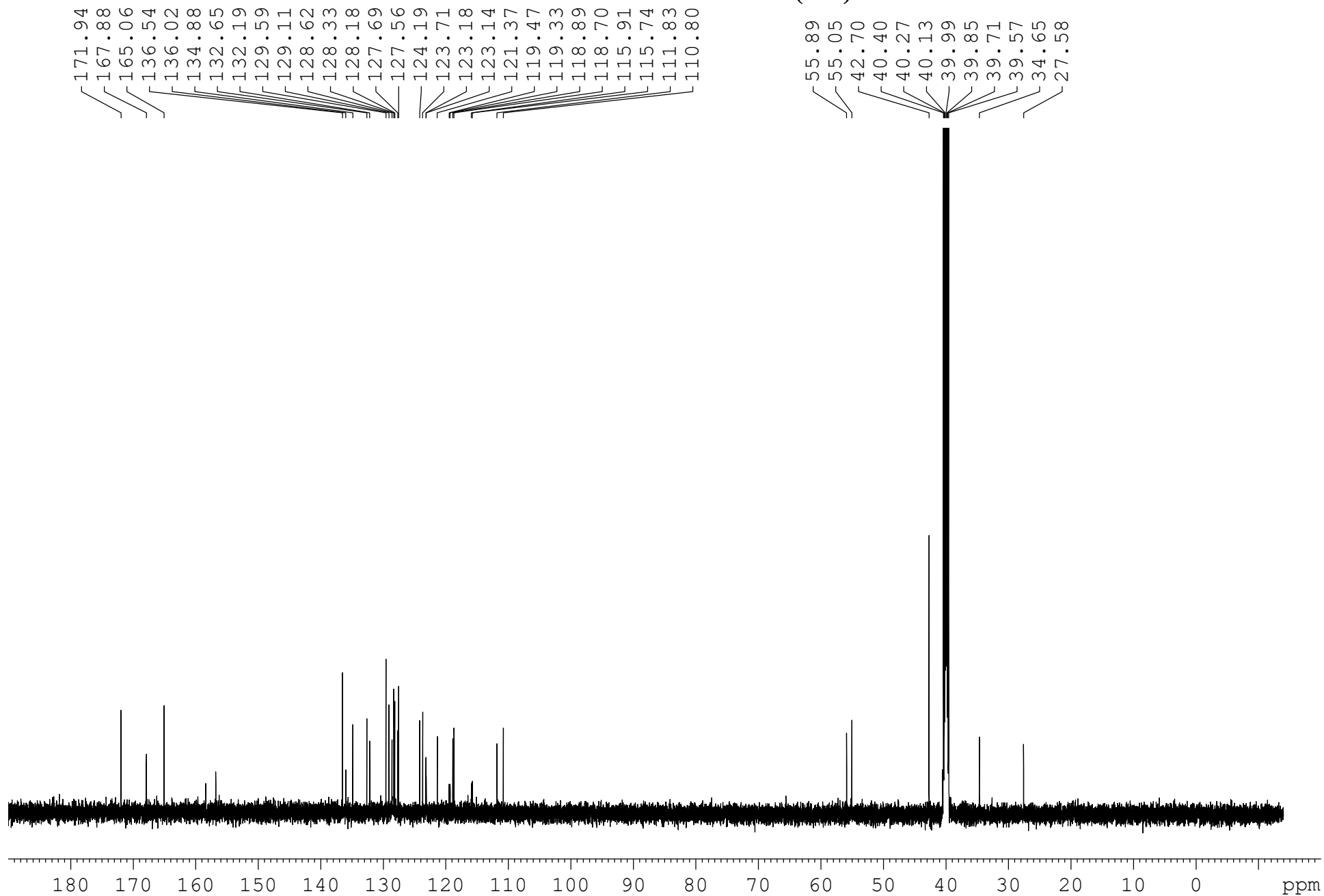
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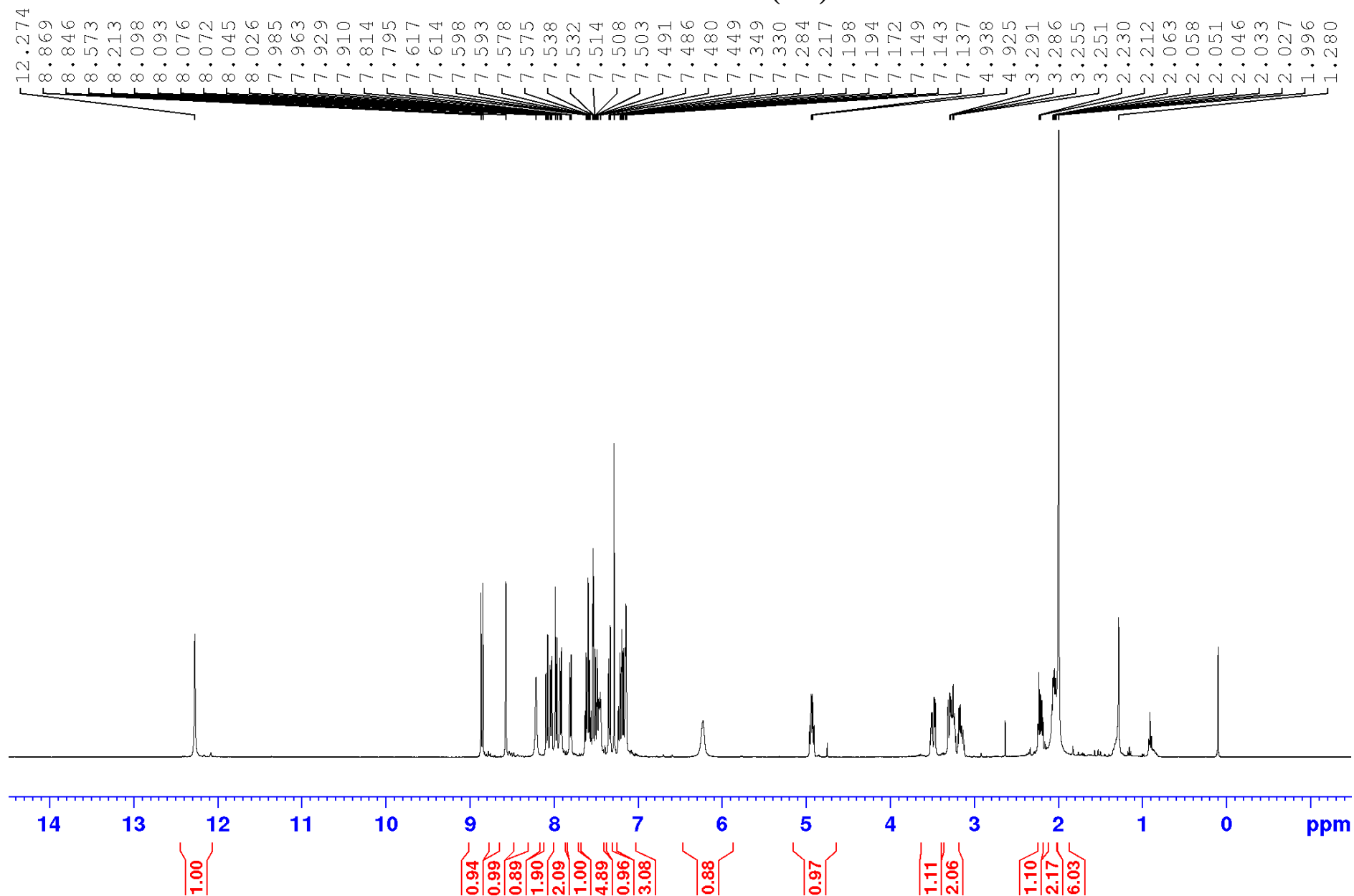
^1H NMR spectra of (*S*)-2-(2-(2-(2-naphthamido)-5-fluorobenzamido)-3-(1*H*-indol-3-yl)propanamido)-*N,N*-dimethylethan-1-aminium chloride (**10b**)



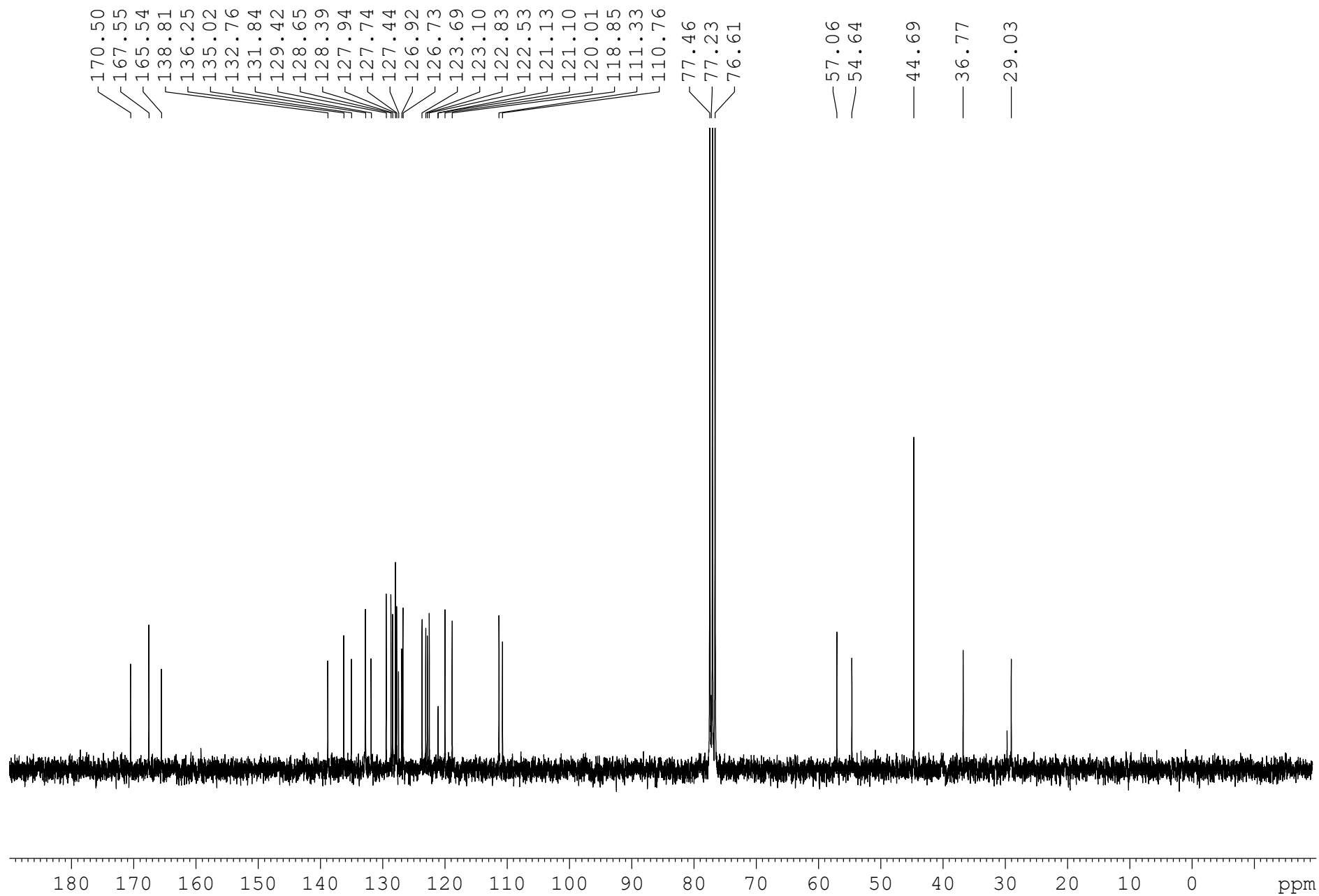
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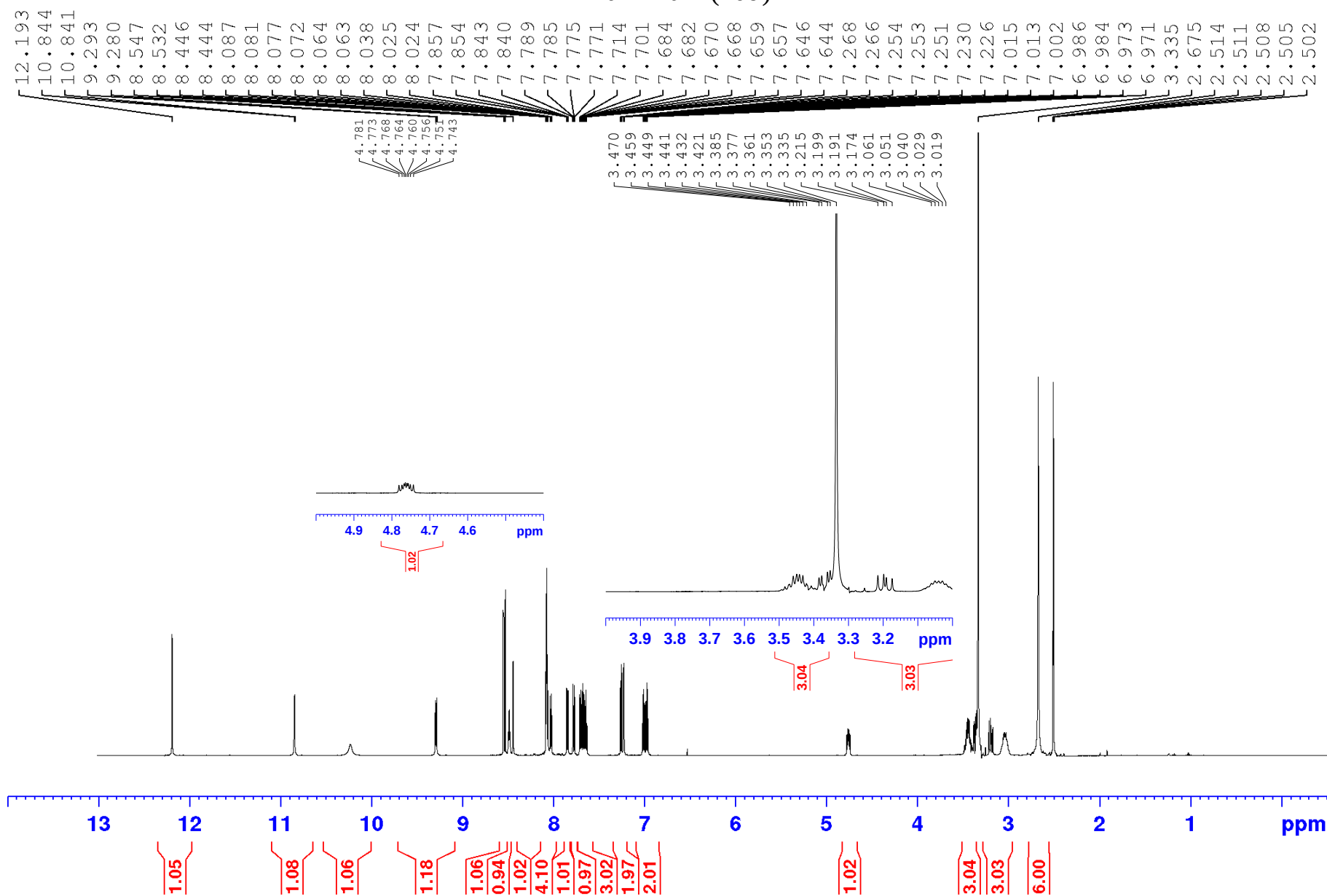
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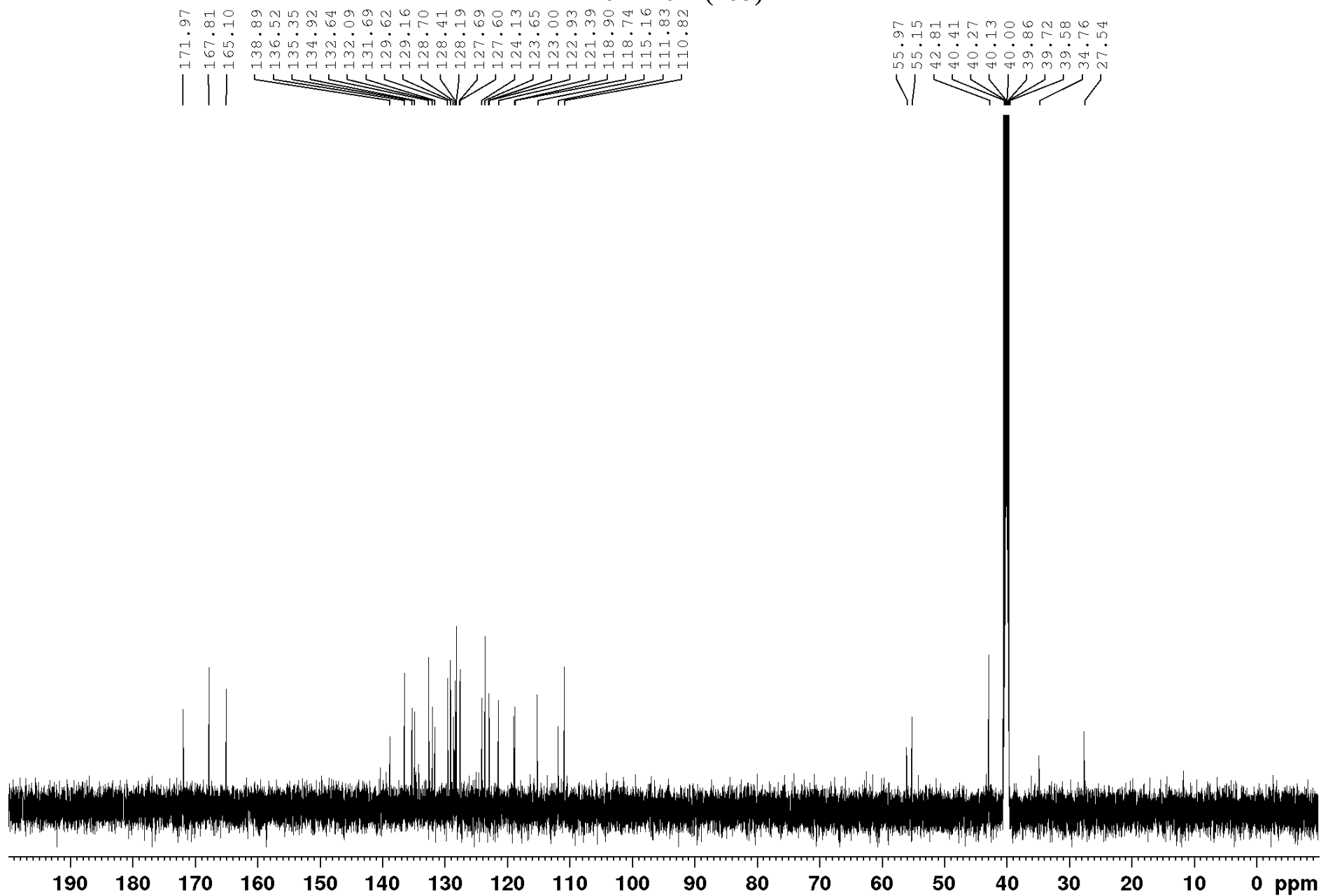
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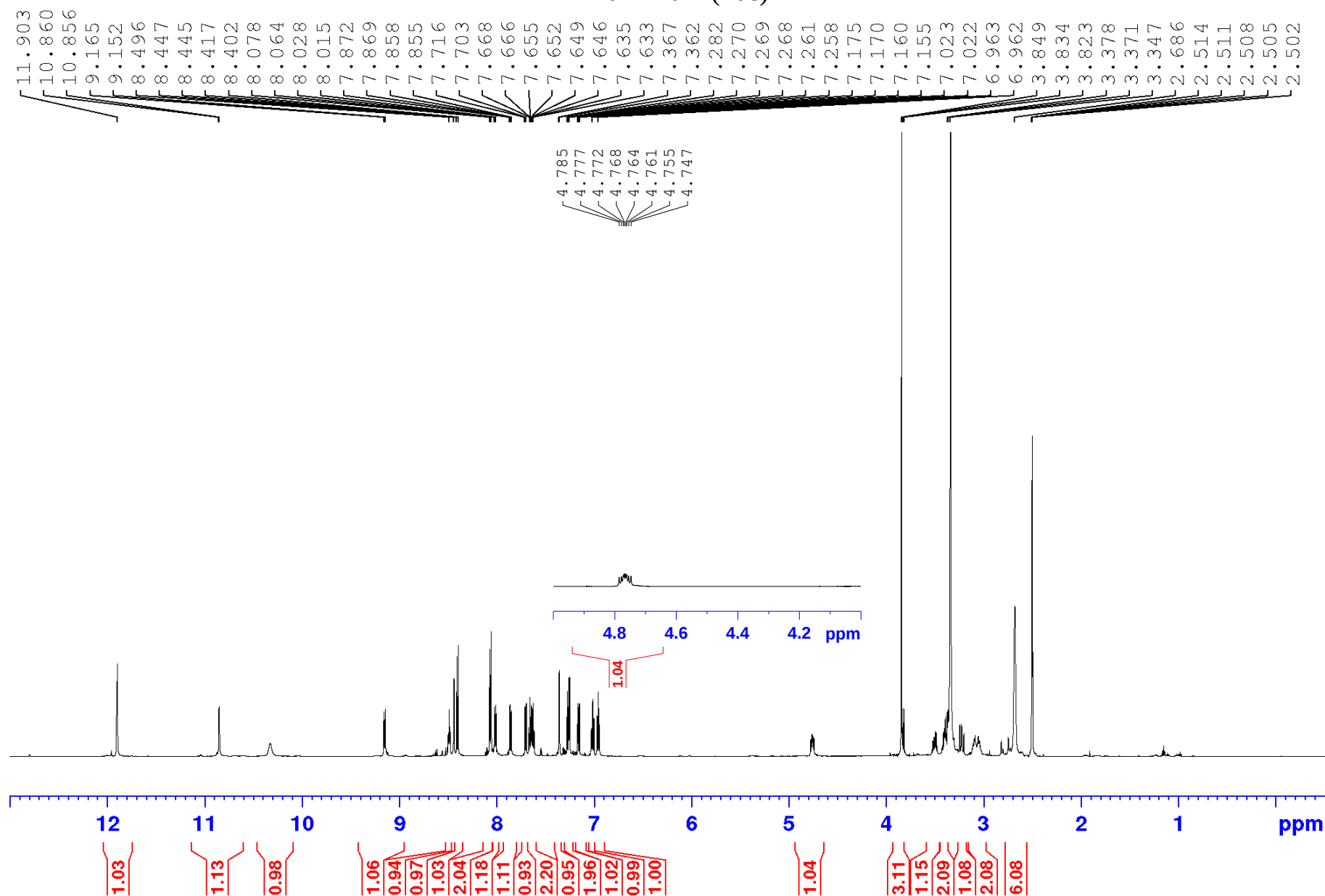
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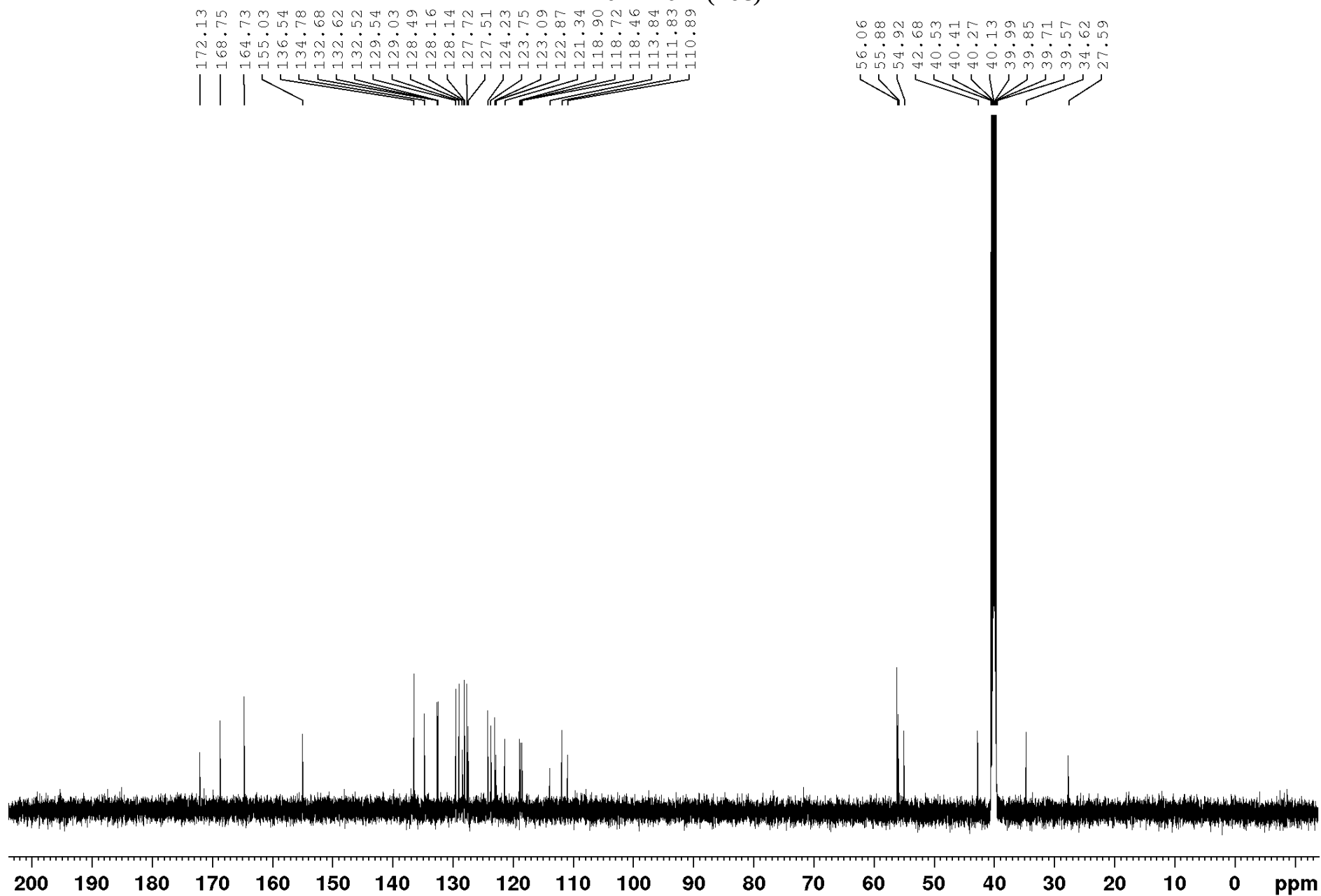
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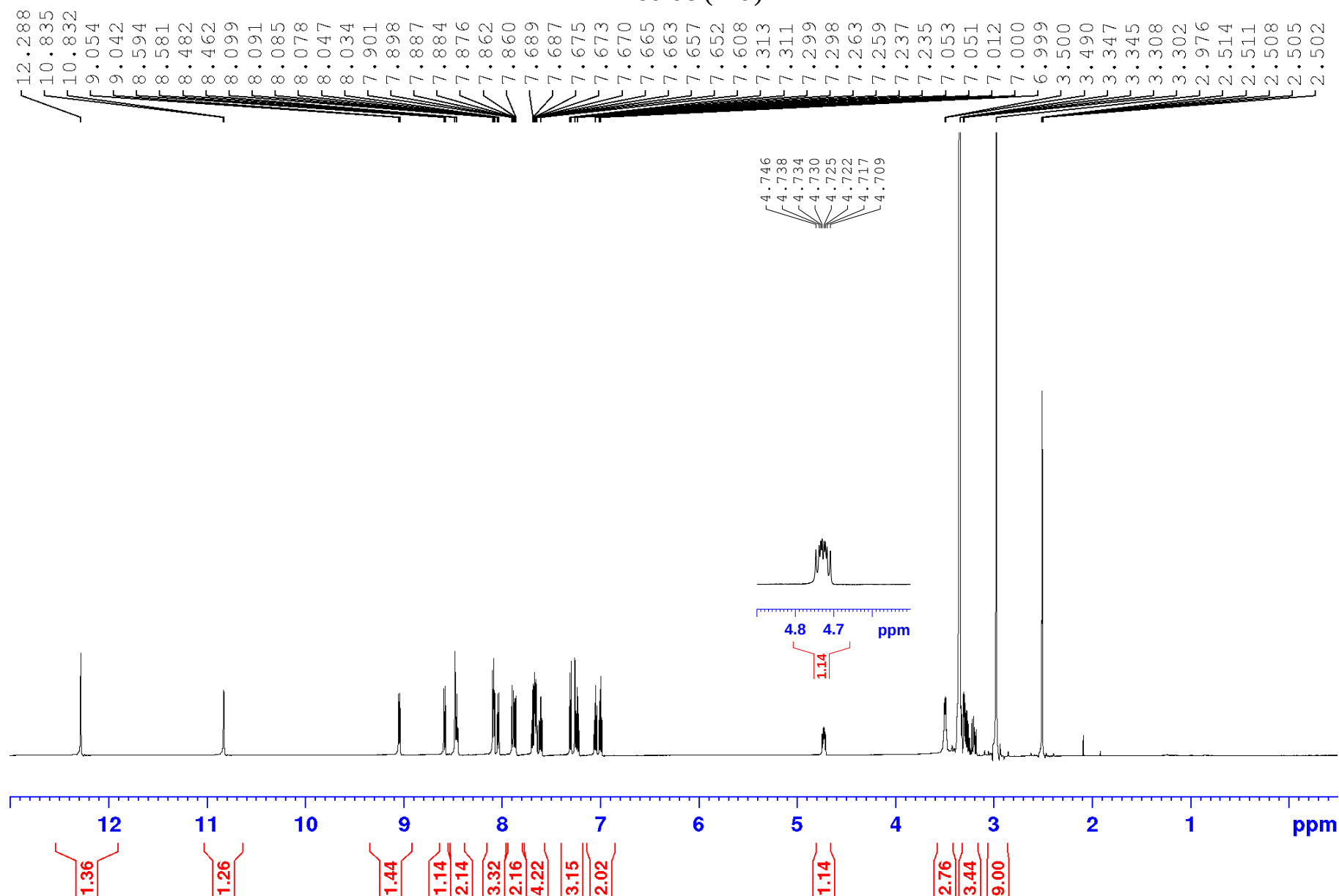
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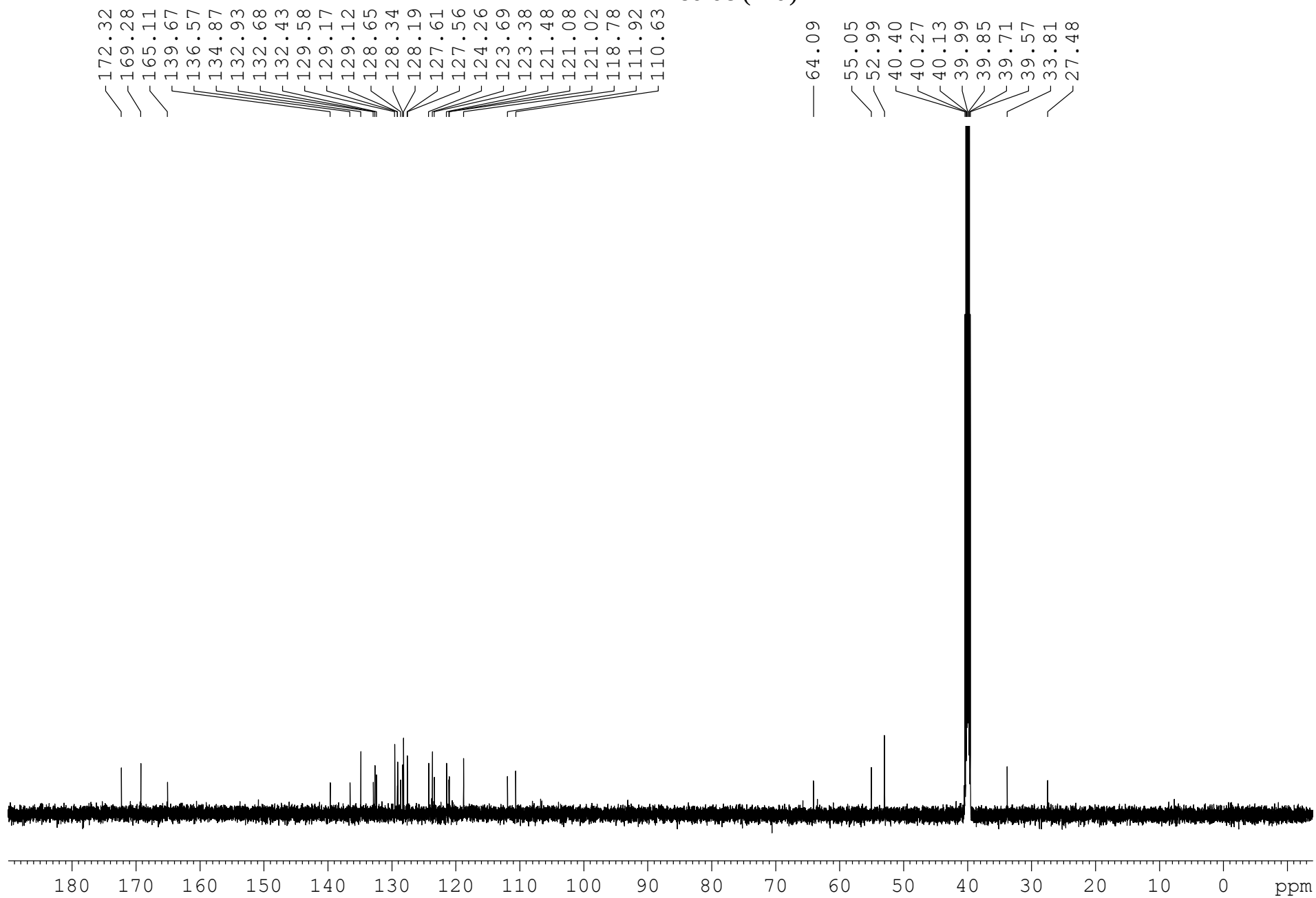
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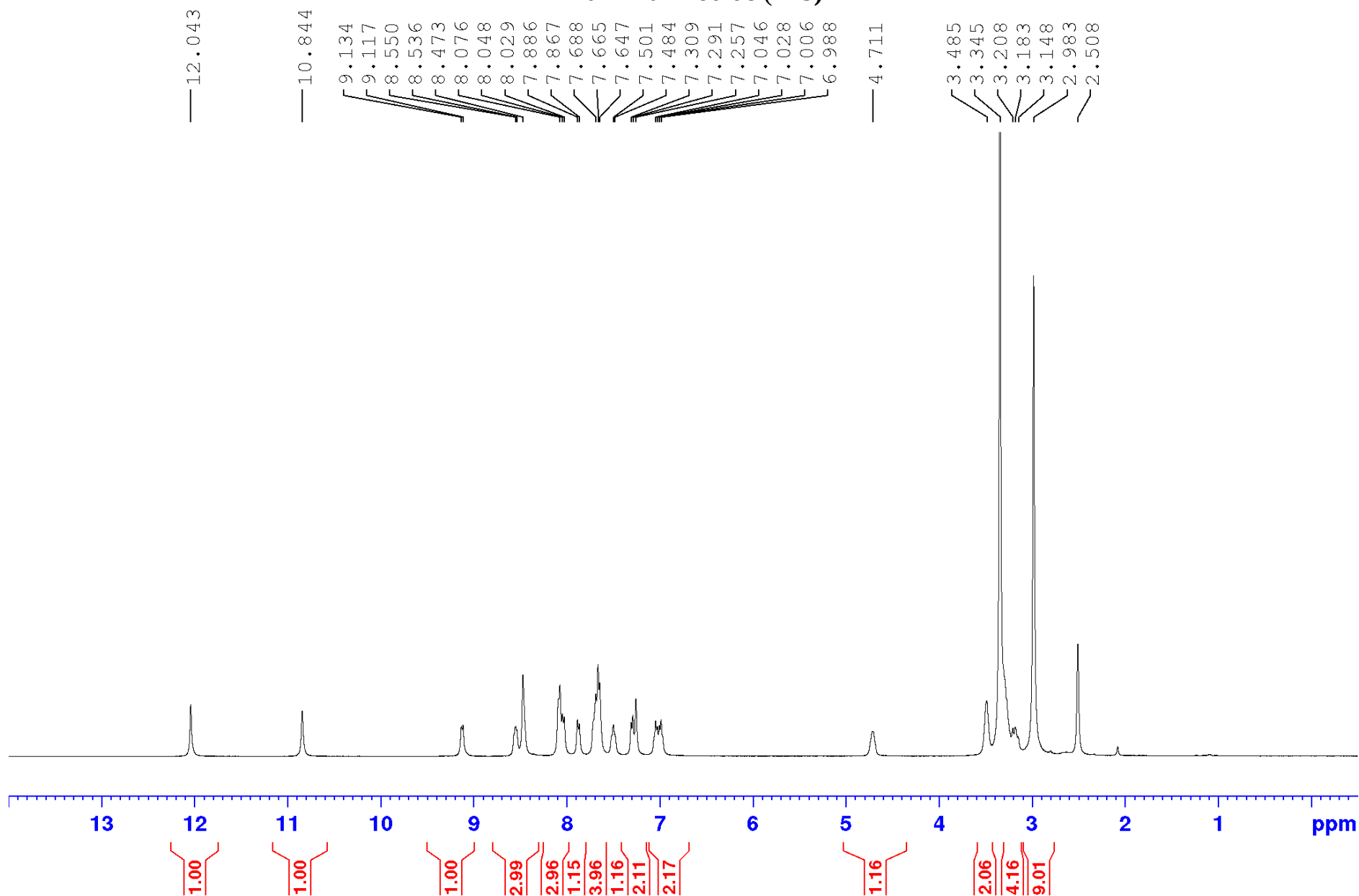
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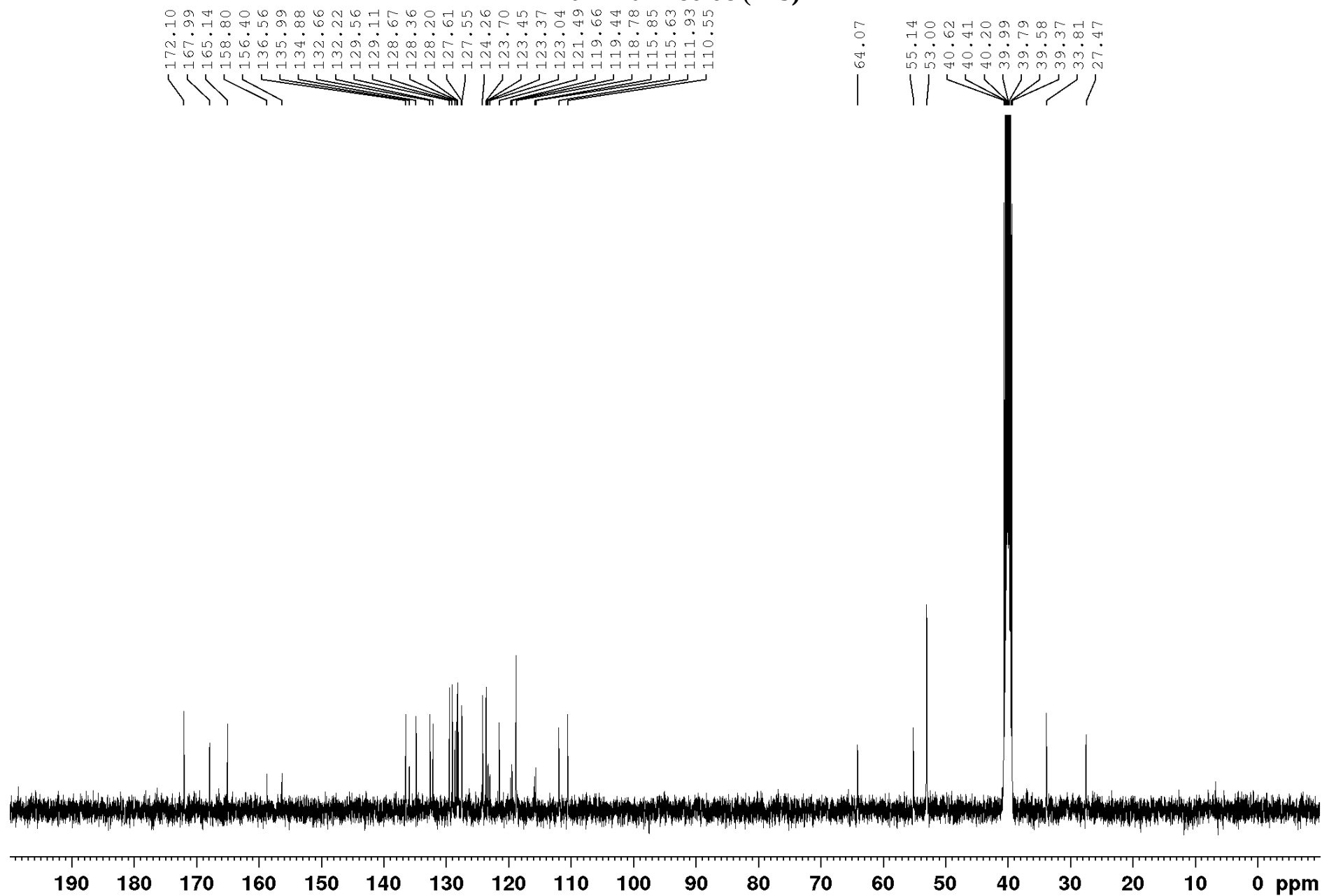
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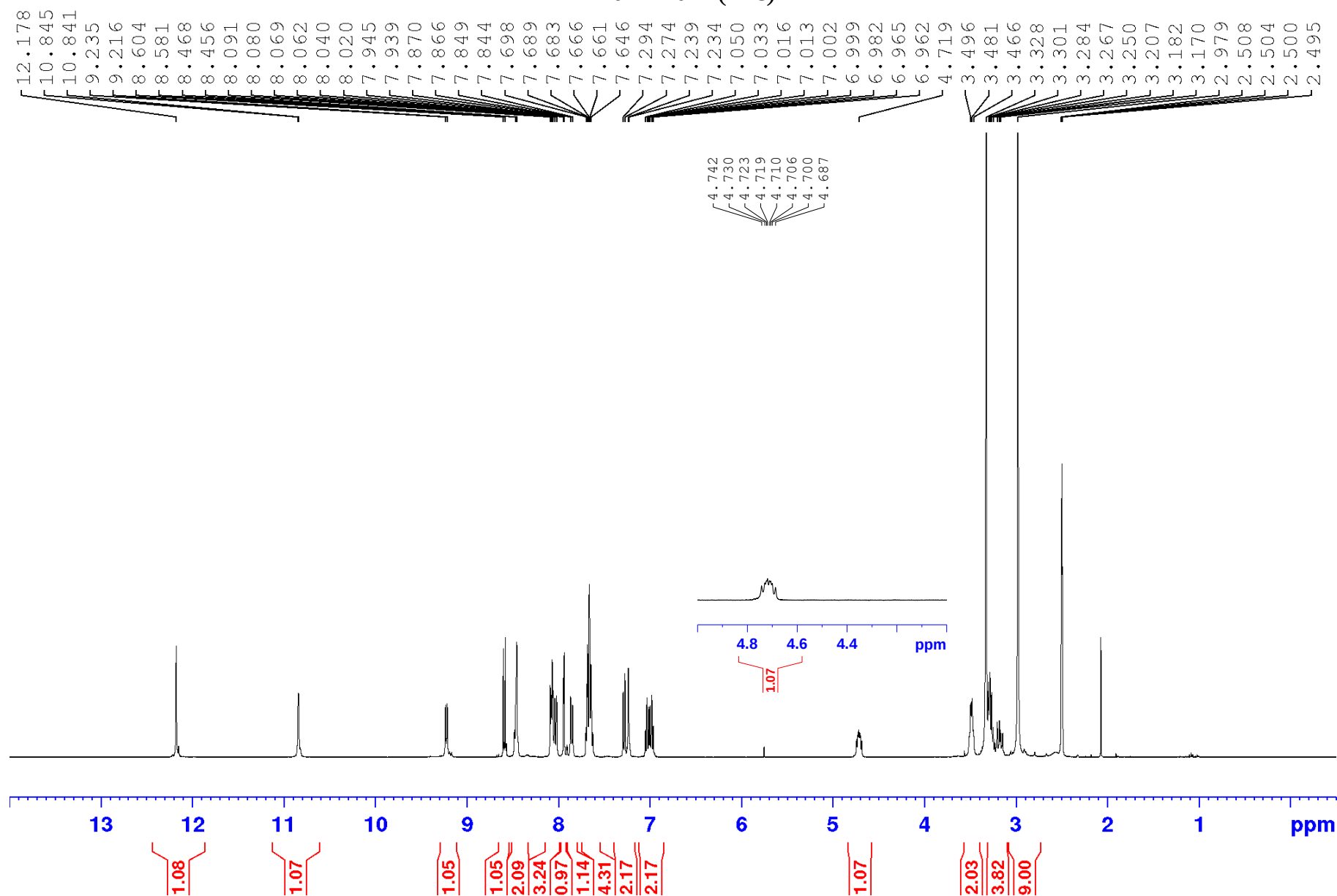
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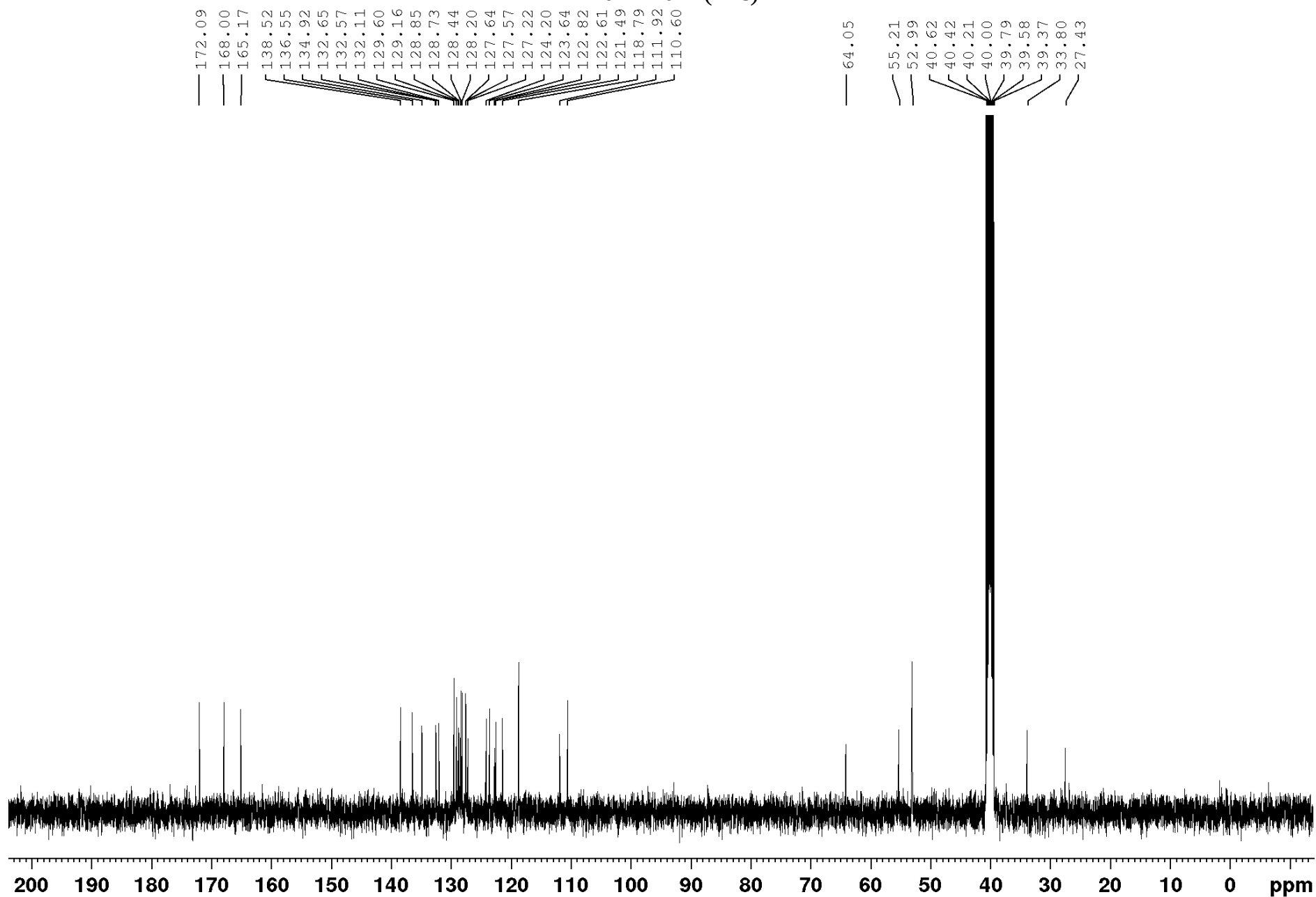
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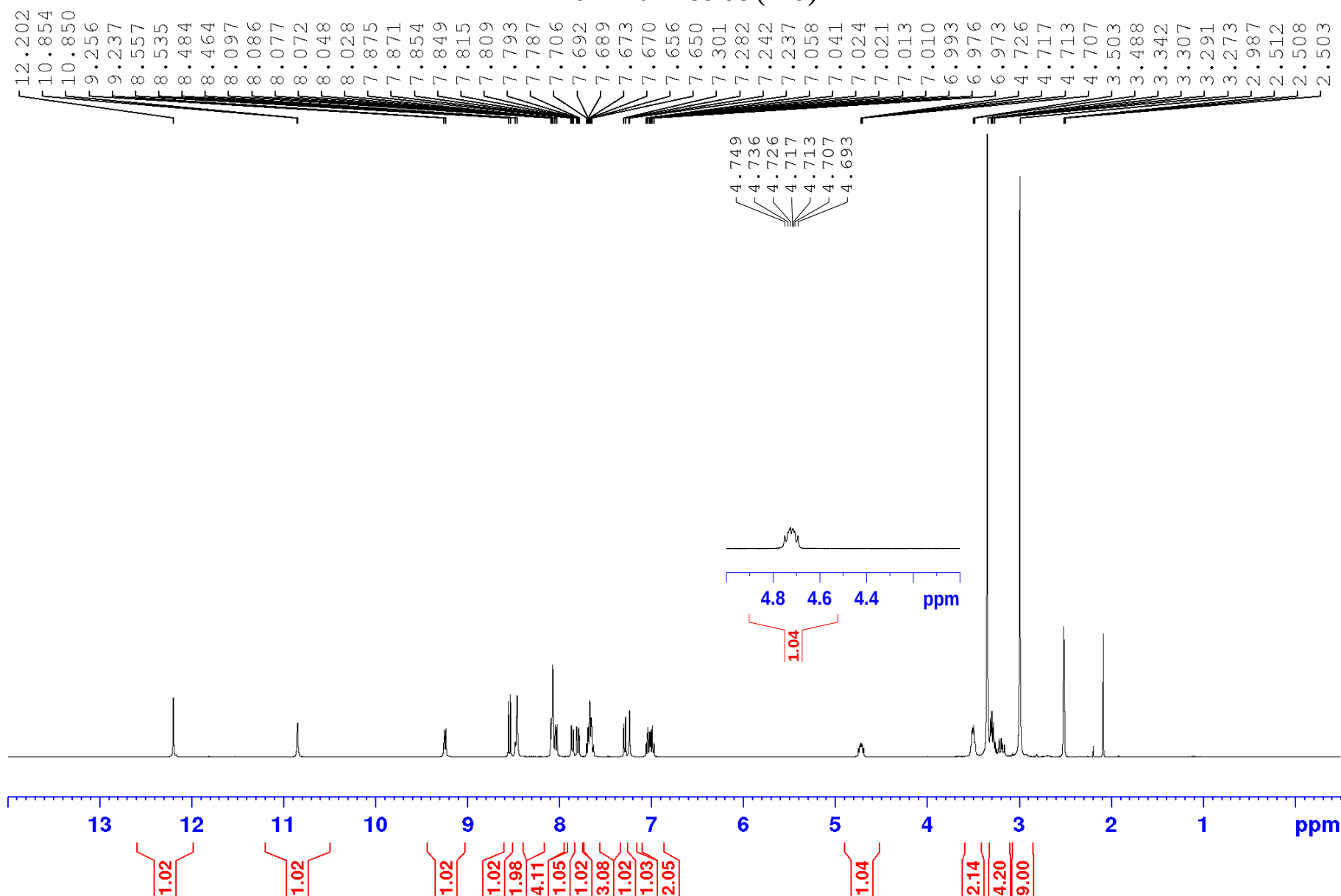
¹H NMR spectra of (S)-2-(2-(2-(2-naphthamido)-5-chlorobenzamido)-3-(1*H*-indol-3-yl)propanamido)-N,N,N-trimethylethan-1-aminium (**11c**)



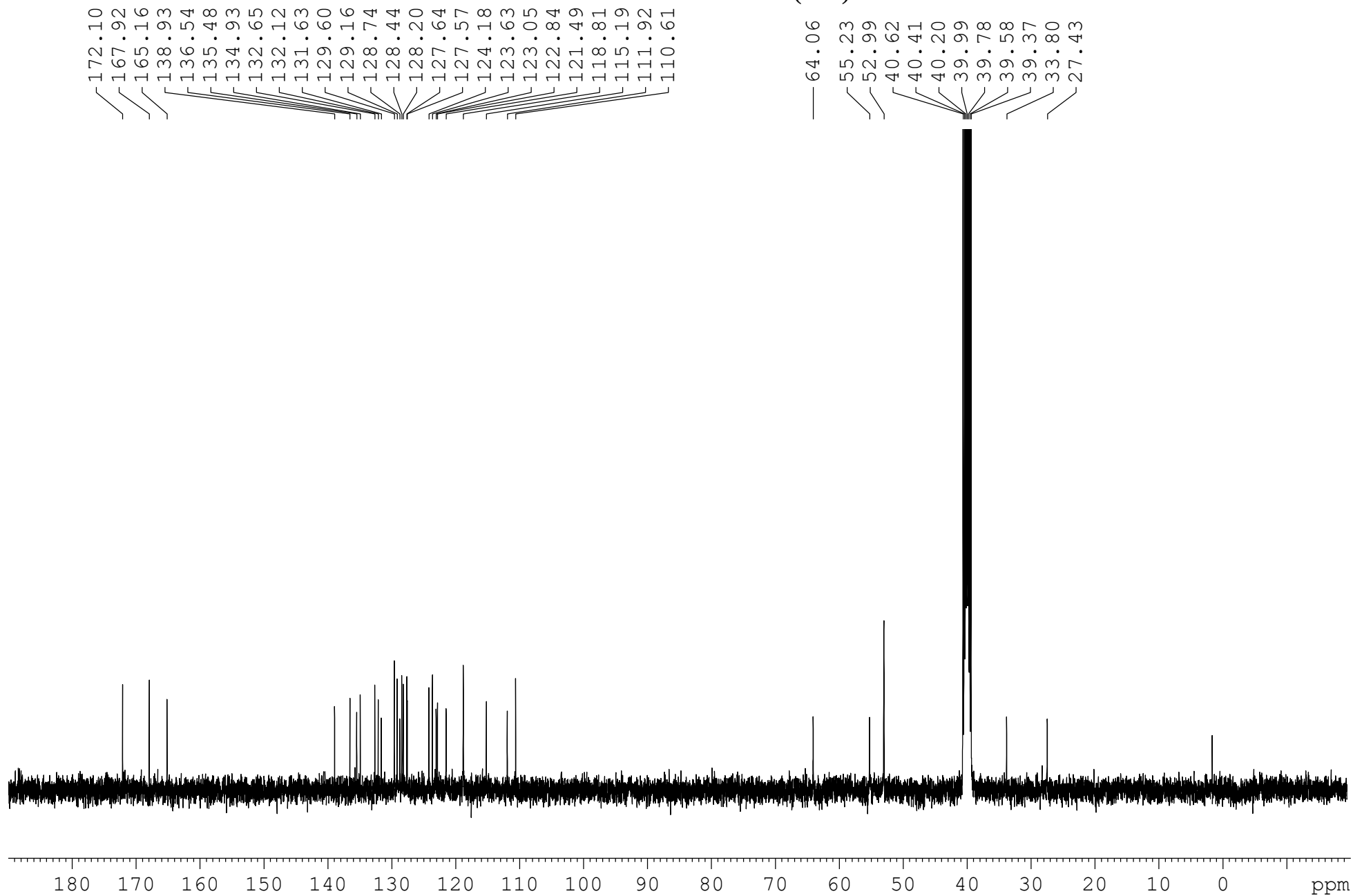
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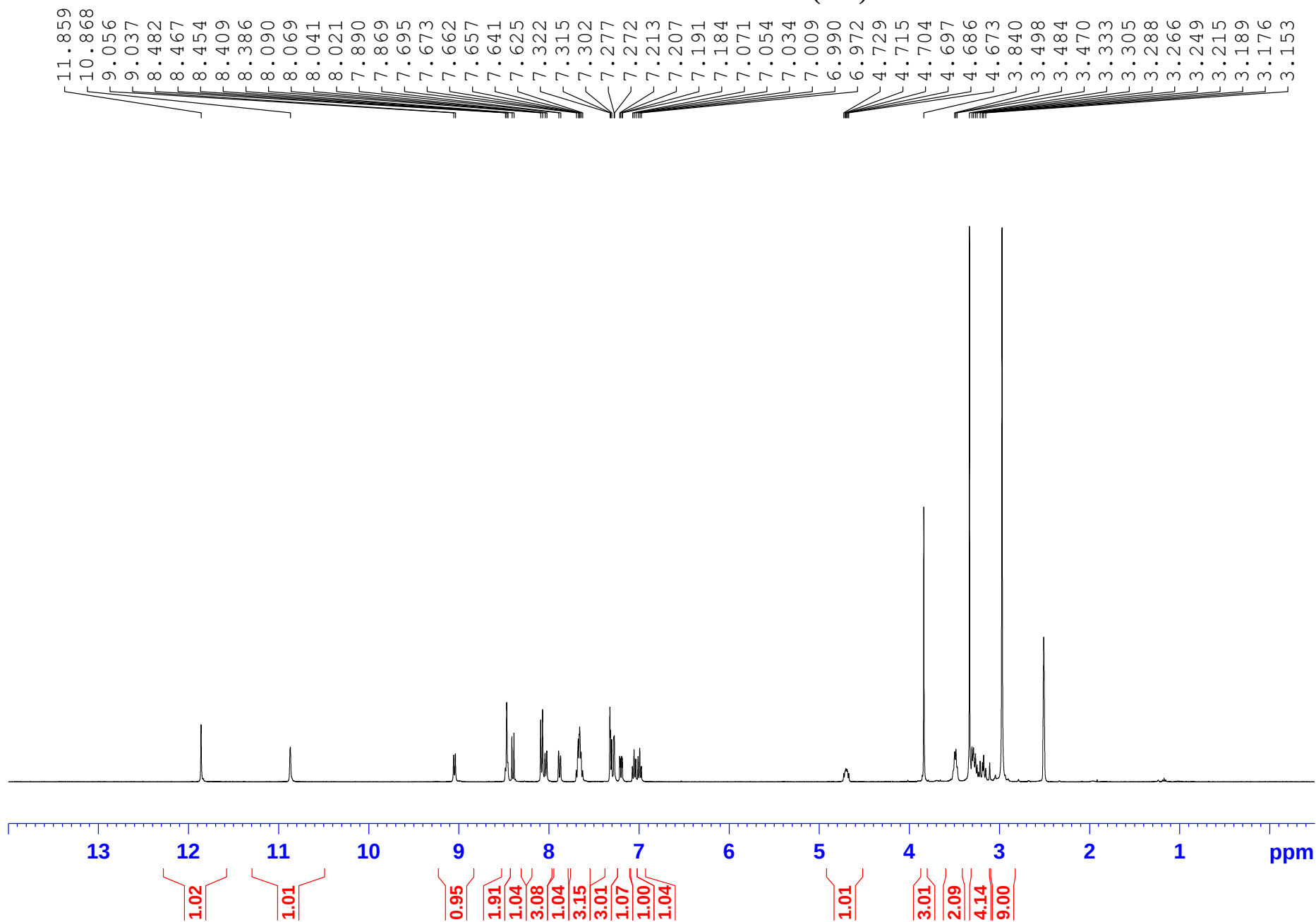
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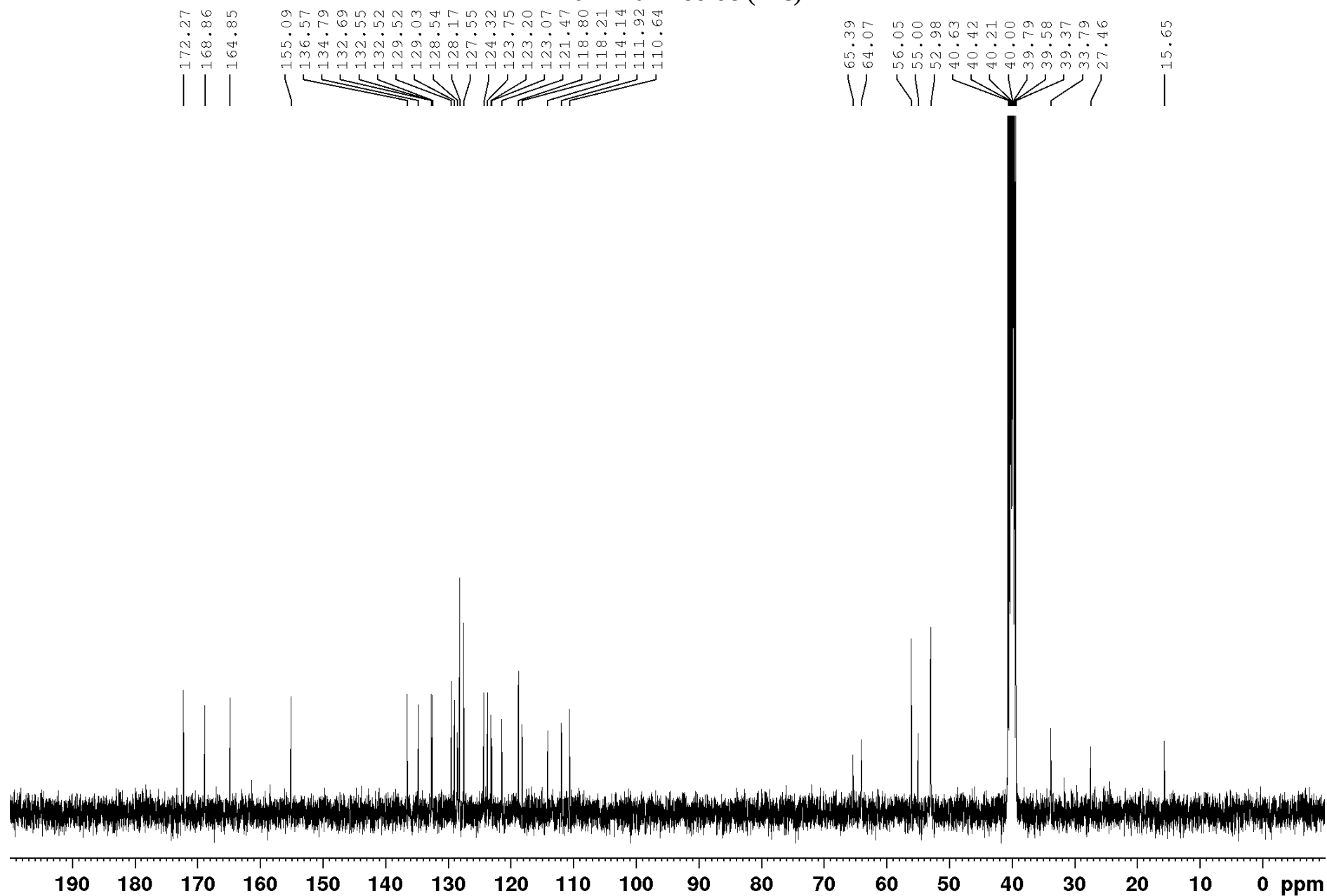
^{13}C NMR spectra of (*S*)-2-(2-(2-(2-naphthamido)-5-bromobenzamido)-3-(1*H*-indol-3-yl)propanamido)-*N,N,N*-trimethylethan-1-aminium iodide (**11d**)



¹H NMR spectra of (S)-2-(2-(2-(2-naphthamido)-5-methoxybenzamido)-3-(1*H*-indol-3-yl)propanamido)-*N,N,N*-trimethylethan-1-aminium iodide (**11e**)



^{13}C NMR spectra of (*S*)-2-(2-(2-(2-naphthamido)-5-methoxybenzamido)-3-(1*H*-indol-3-yl)propanamido)-*N,N,N*-trimethylethan-1-aminium iodide (**11e**)



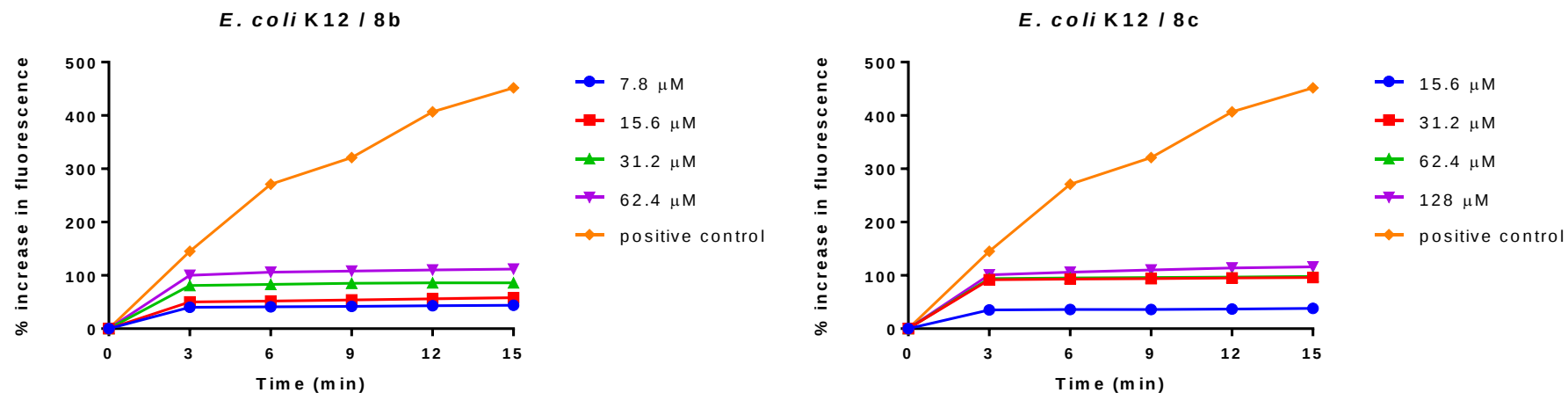


Fig. S1: *E. coli* cytoplasmic membrane disruption promoted by **8b** and **8c** at different concentrations. 20% DMSO used as positive control

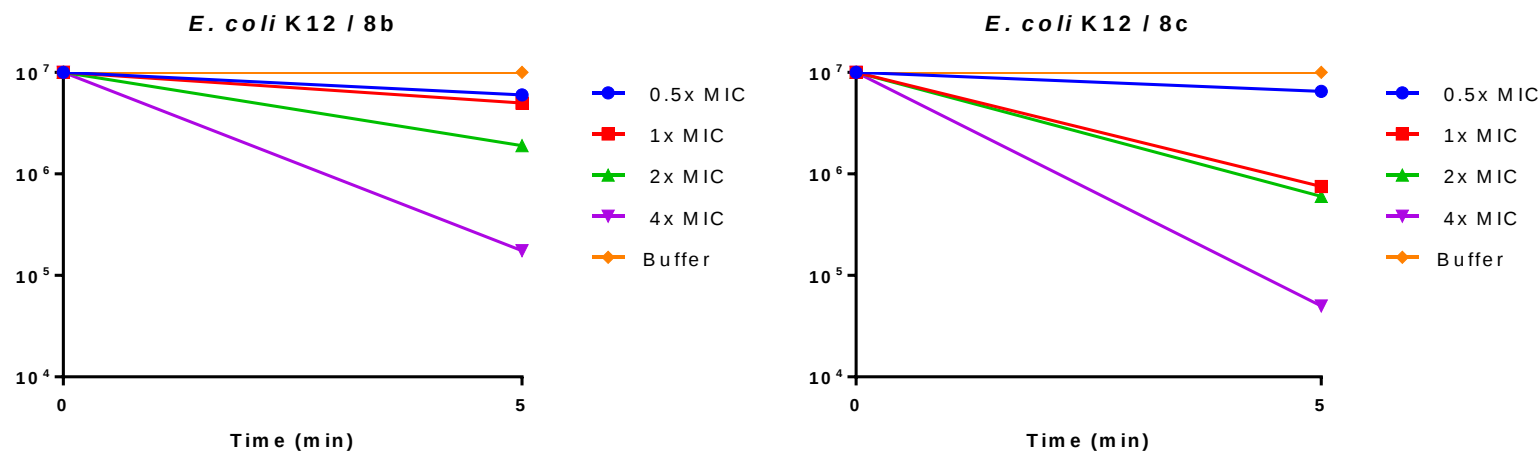


Fig. S2: *E. coli* cell viability count of 8b and 8c at different concentrations.

Fig. S3: Disruption of established biofilm of *S. aureus* after 24 h with 1 $\times$ to 32 $\times$ MIC concentrations of compound **10d**.

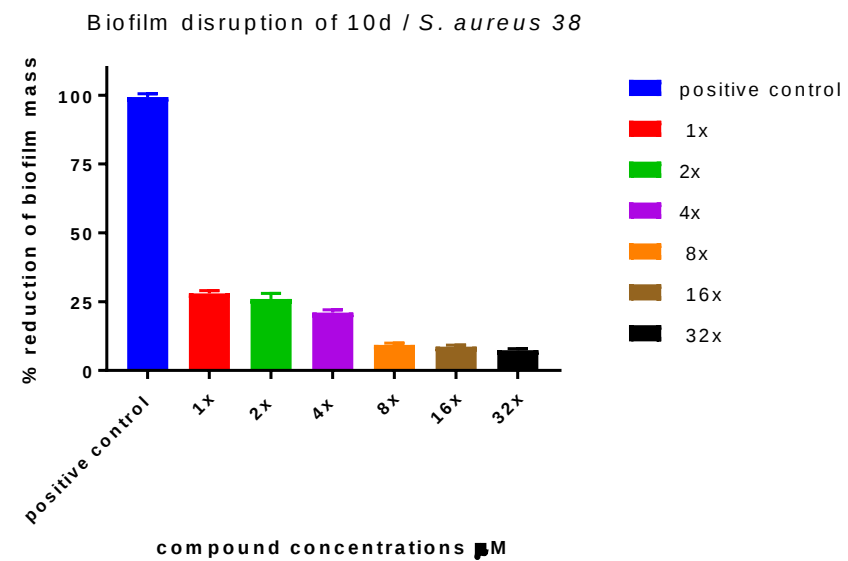


Fig. S3: Disruption of established biofilm of *S. aureus* after 24 h with 1 $\times$ to 32 $\times$ MIC concentrations of compound **10d**.