

Supporting Information:

Nicotinic Acid Adenine Dinucleotide Phosphate Analogs Containing Substituted

Nicotinic Acid: Effect of Modification on Ca²⁺ Release

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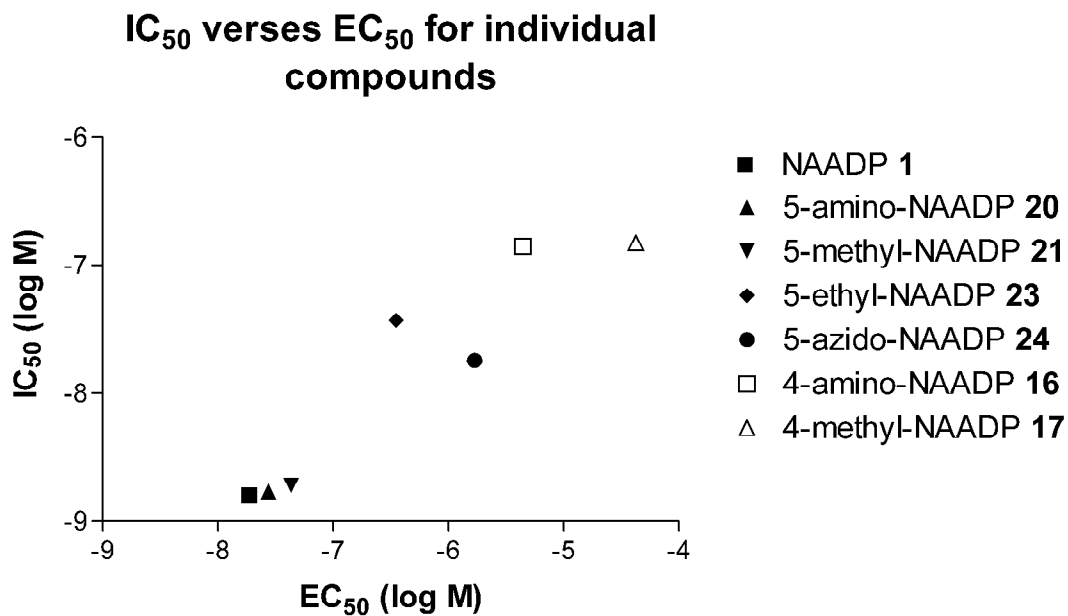


Figure S1. Scatter plot of the IC₅₀ values derived from competition ligand binding (Table 4)(Y-axis) versus the EC₅₀ values derived from Ca²⁺ release (Table 3)(X-axis).

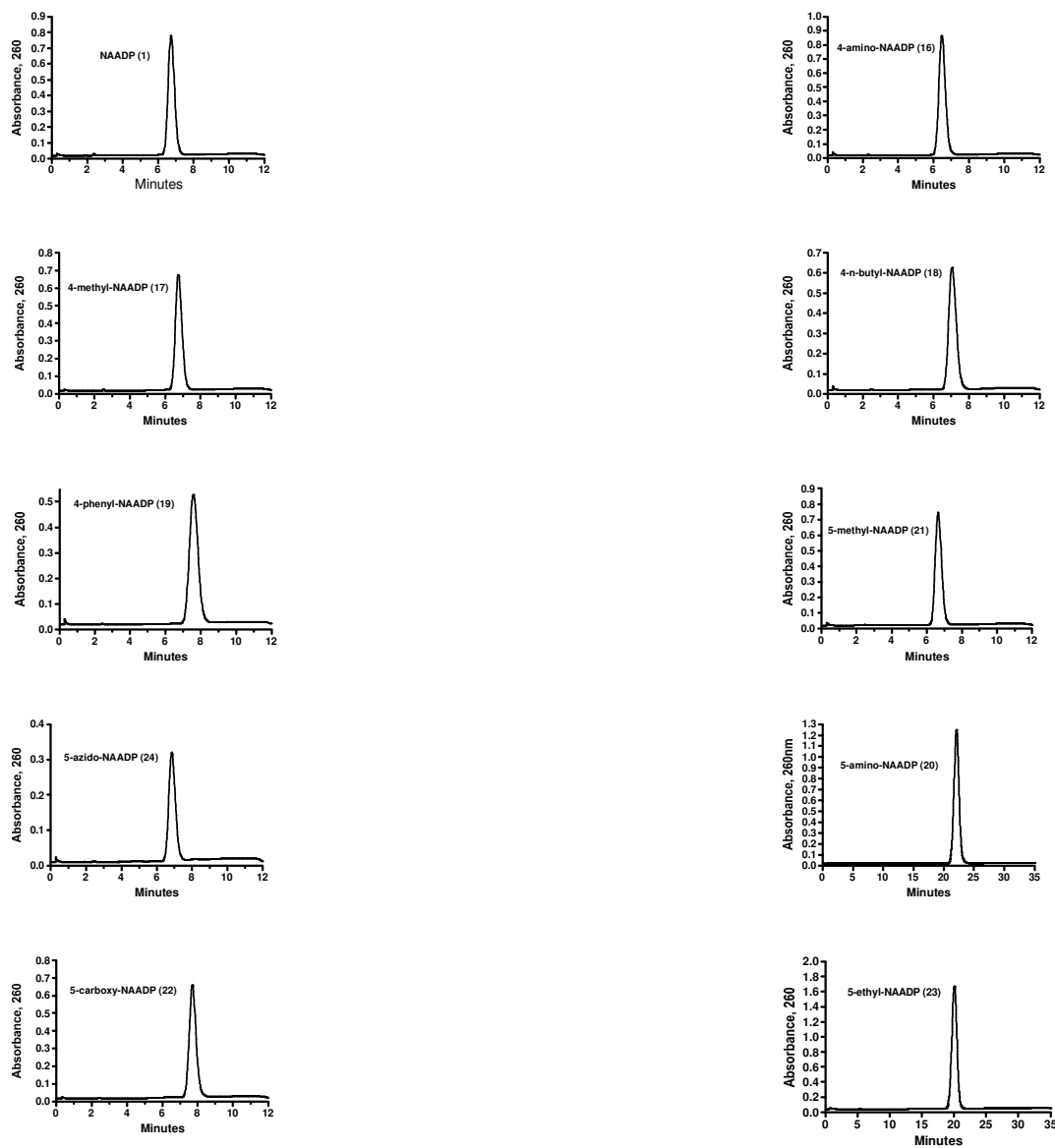


Figure S2. HPLC of NAADP and its analogs **16 – 24**. Compounds were examined using high pressure liquid chromatography (HPLC) on a 4.6×50 mm column packed with AG MP-1 macroporus anion exchange resin (BioRad Laboratories) with the chromatography developed at 1 mL/min using a mobile phase of 0 – 75 mM trifluoroacetic acid in water¹ immediately prior to testing.

Figure S3. $^1\text{H-NMR}$ (400 MHz, CD_3OD) 4-*n*-butylnicotinic acid

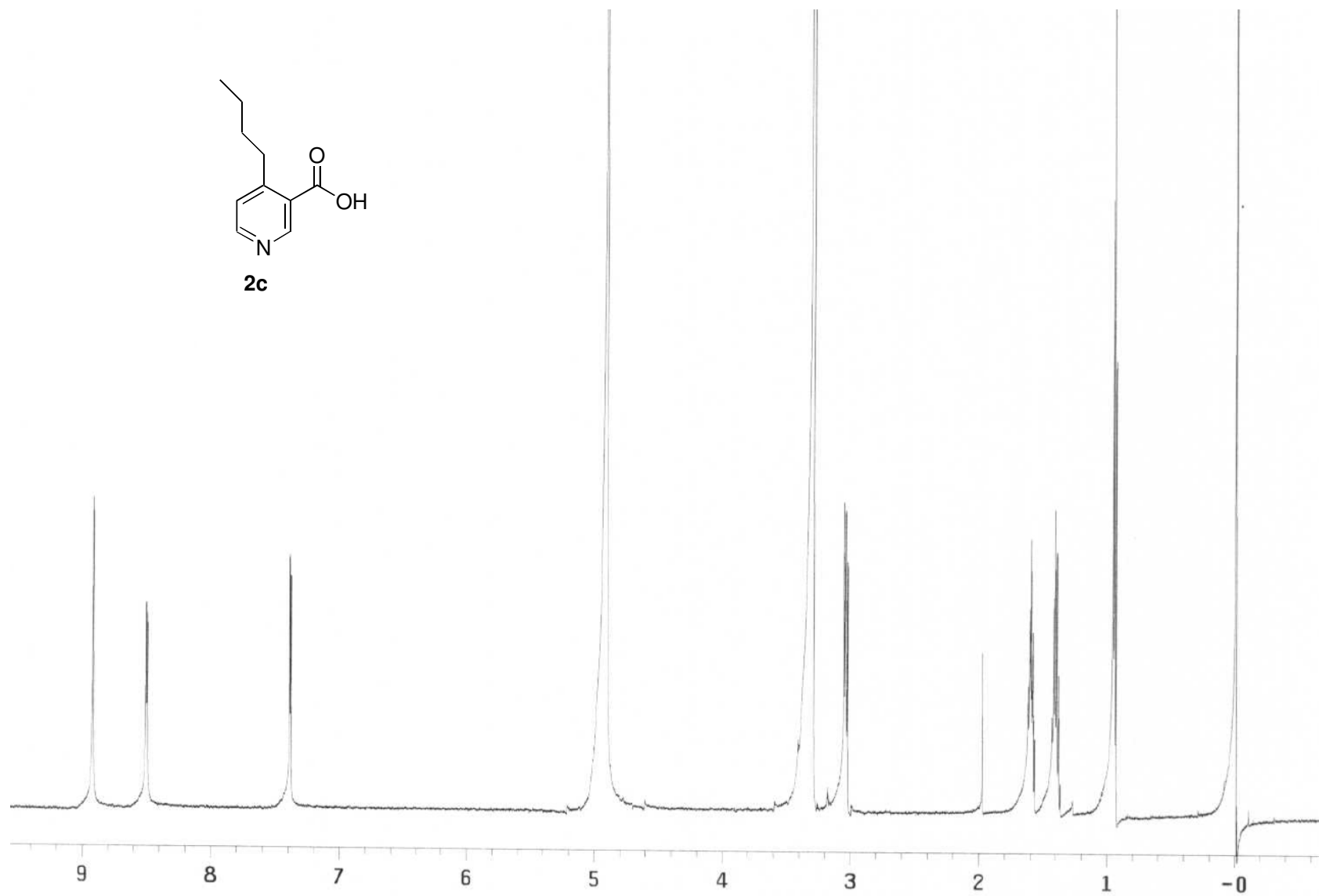


Figure S4. ¹H-NMR (400 MHz, CDCl₃) 4-phenylnicotinic acid.

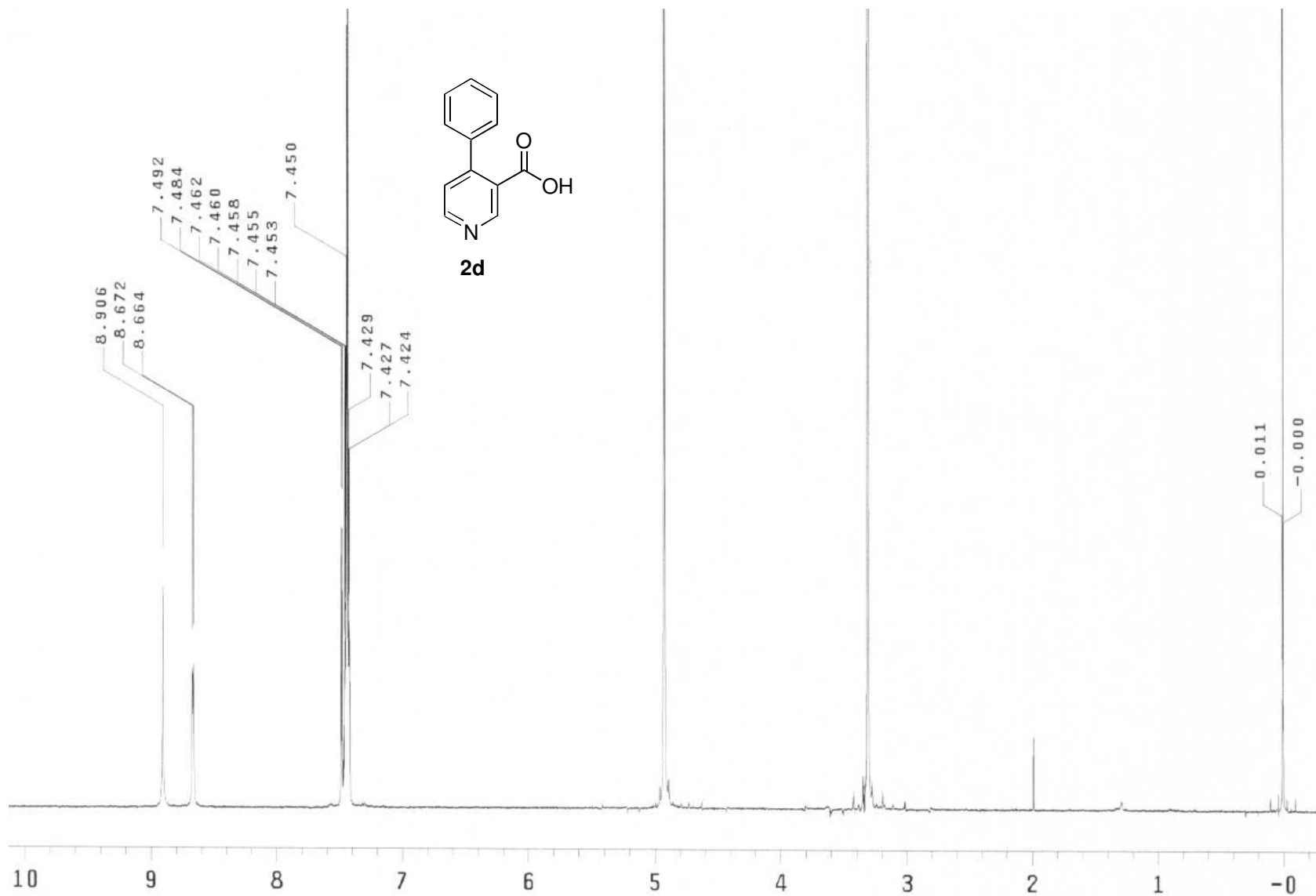


Figure S5. $^1\text{H-NMR}$ (400 MHz, CD_3OD) 5-ethynynicotinic acid (**3e**).

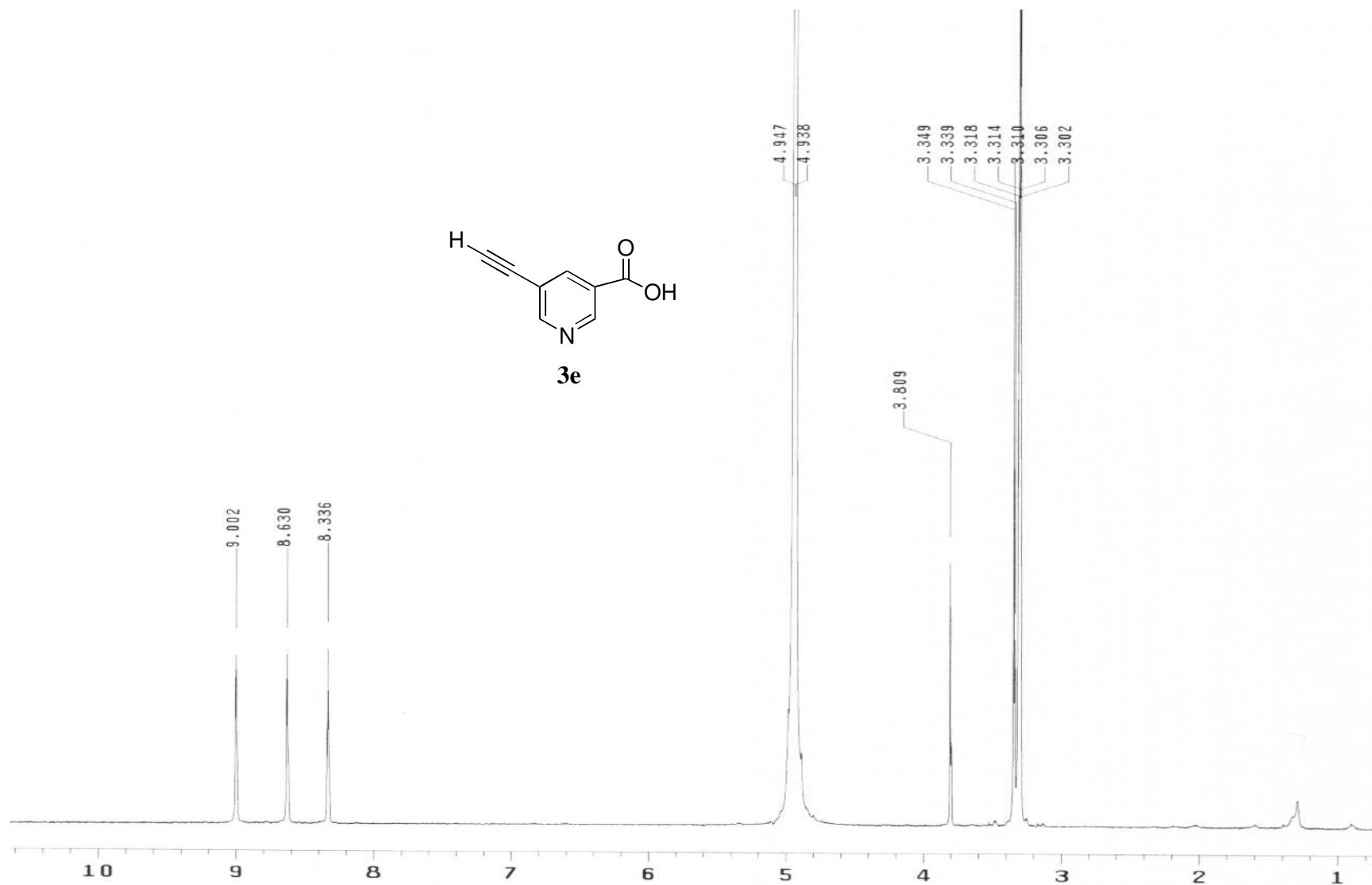


Figure S6. ^{13}C -NMR (CD_3OD) 5-ethynynicotinic acid (**3e**).

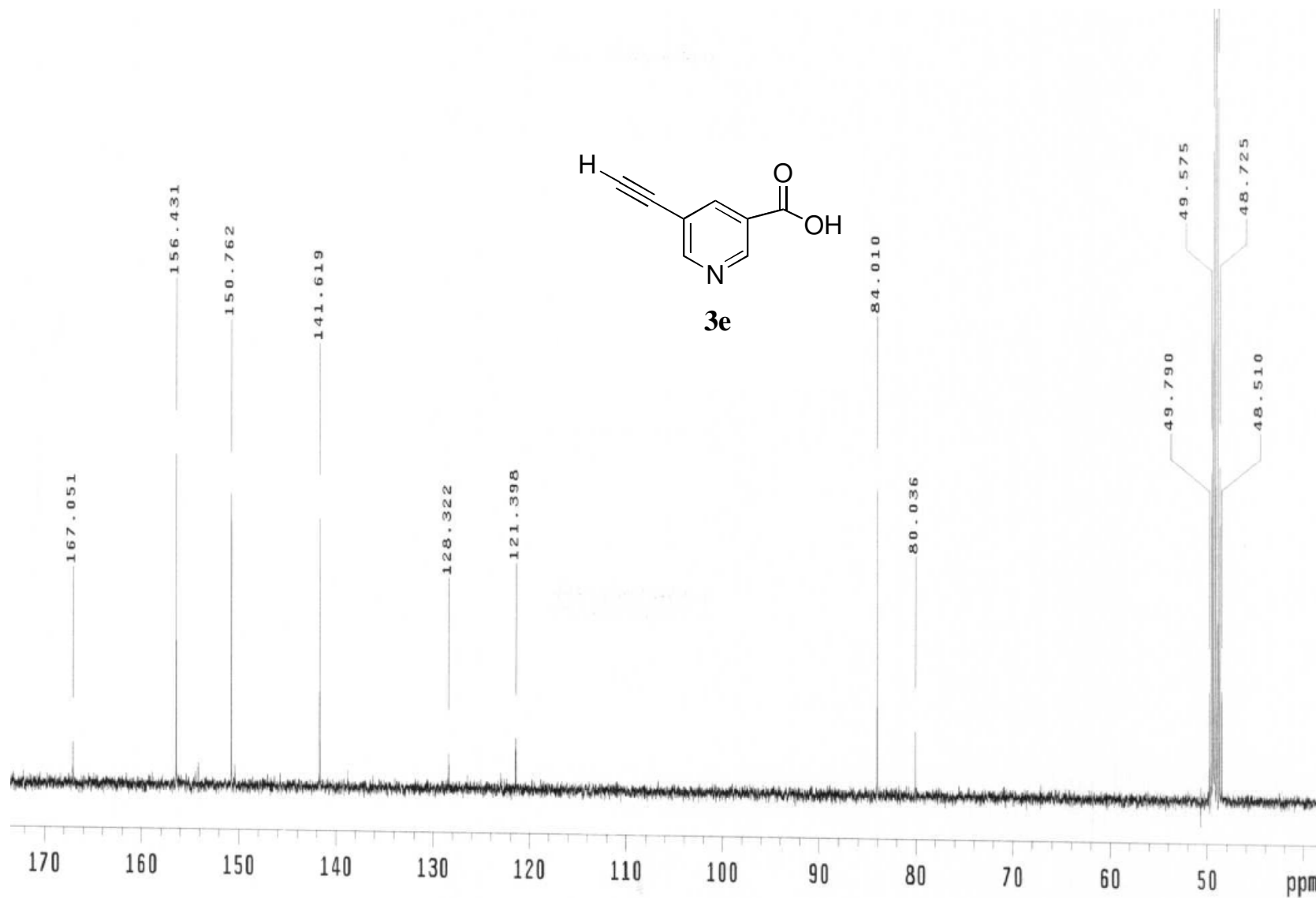


Figure S7. $^1\text{H-NMR}$ of **3f**: 5-ethenylnicotinic acid

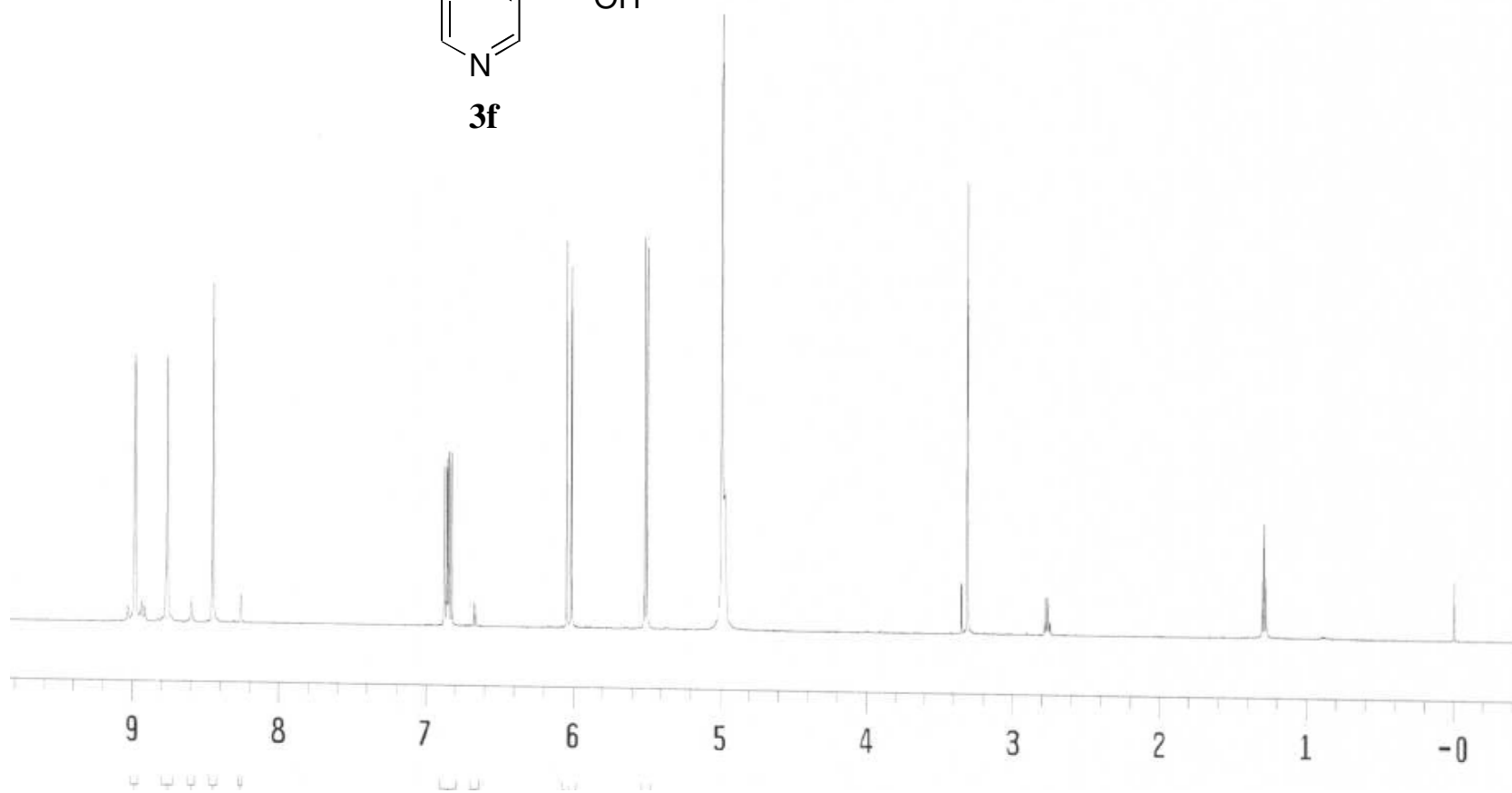
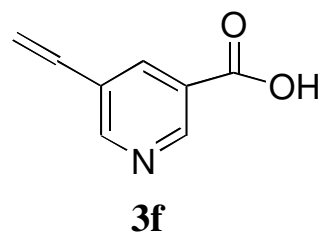


Figure S8. ^{13}C -NMR of **3f**: 5-ethynynicotinic acid

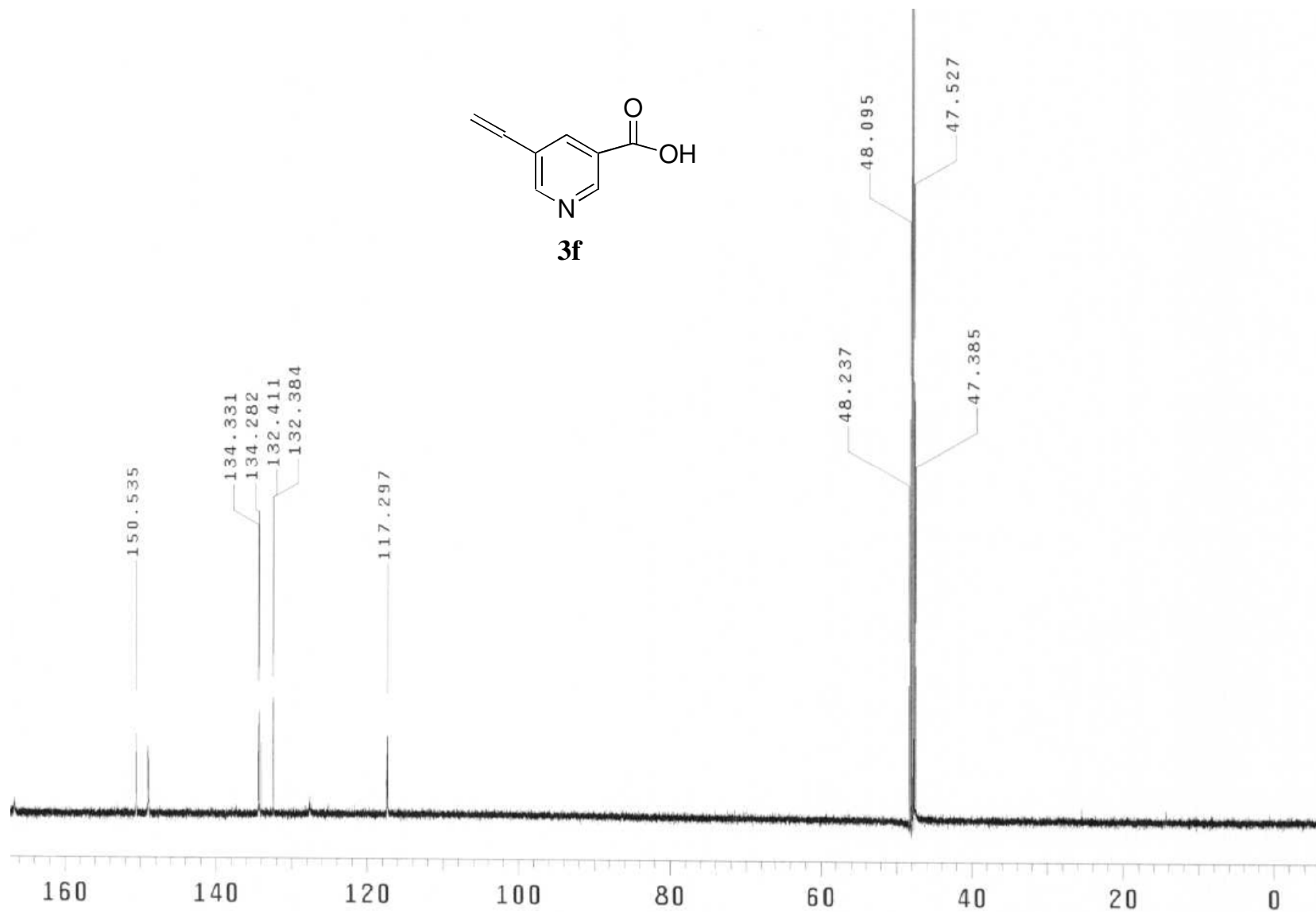


Figure S9. ¹H-NMR of **3g**: 5-ethylnicotinic acid

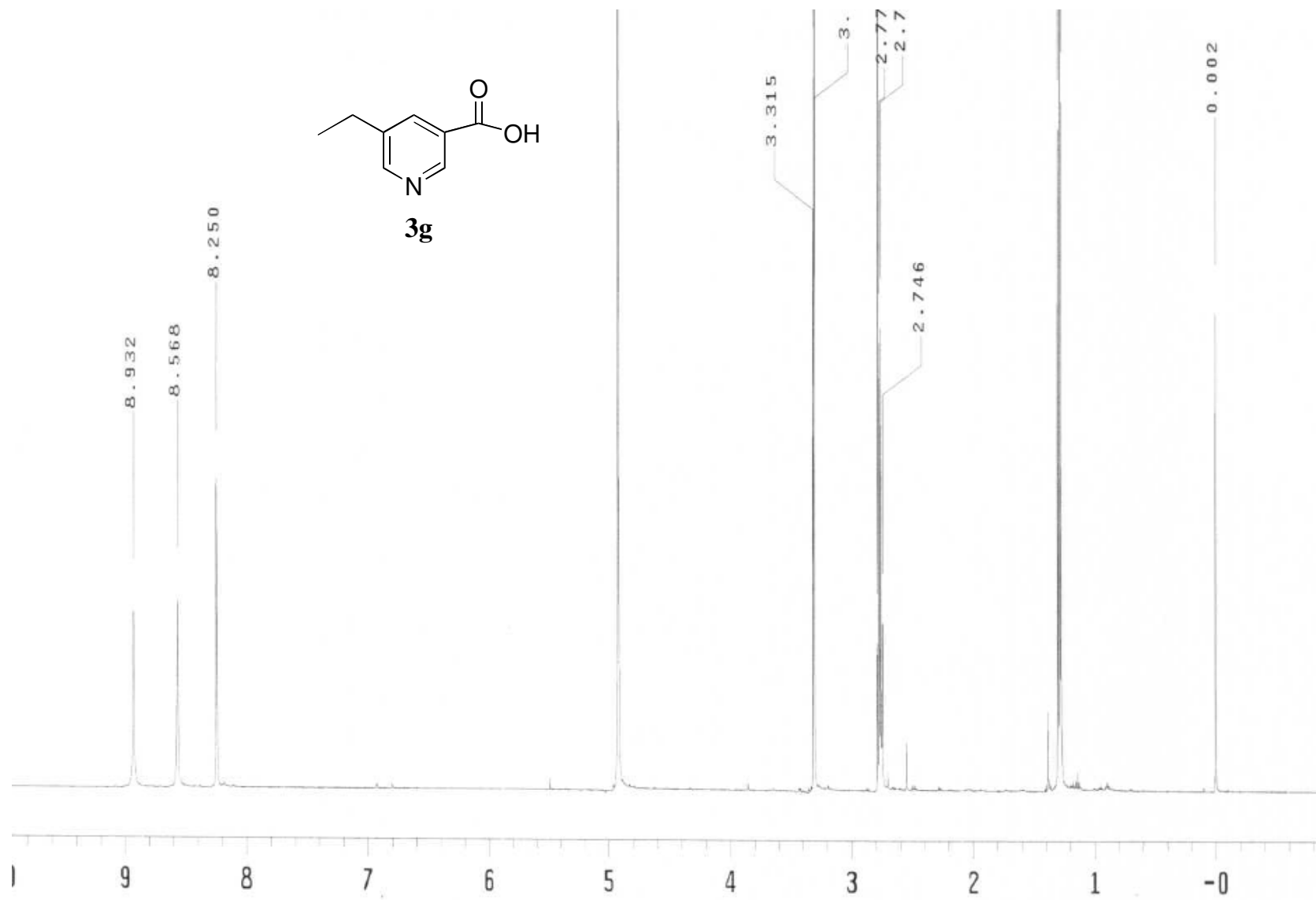


Figure S10. ^{13}C -NMR of **3g**: 5-ethylnicotinic acid

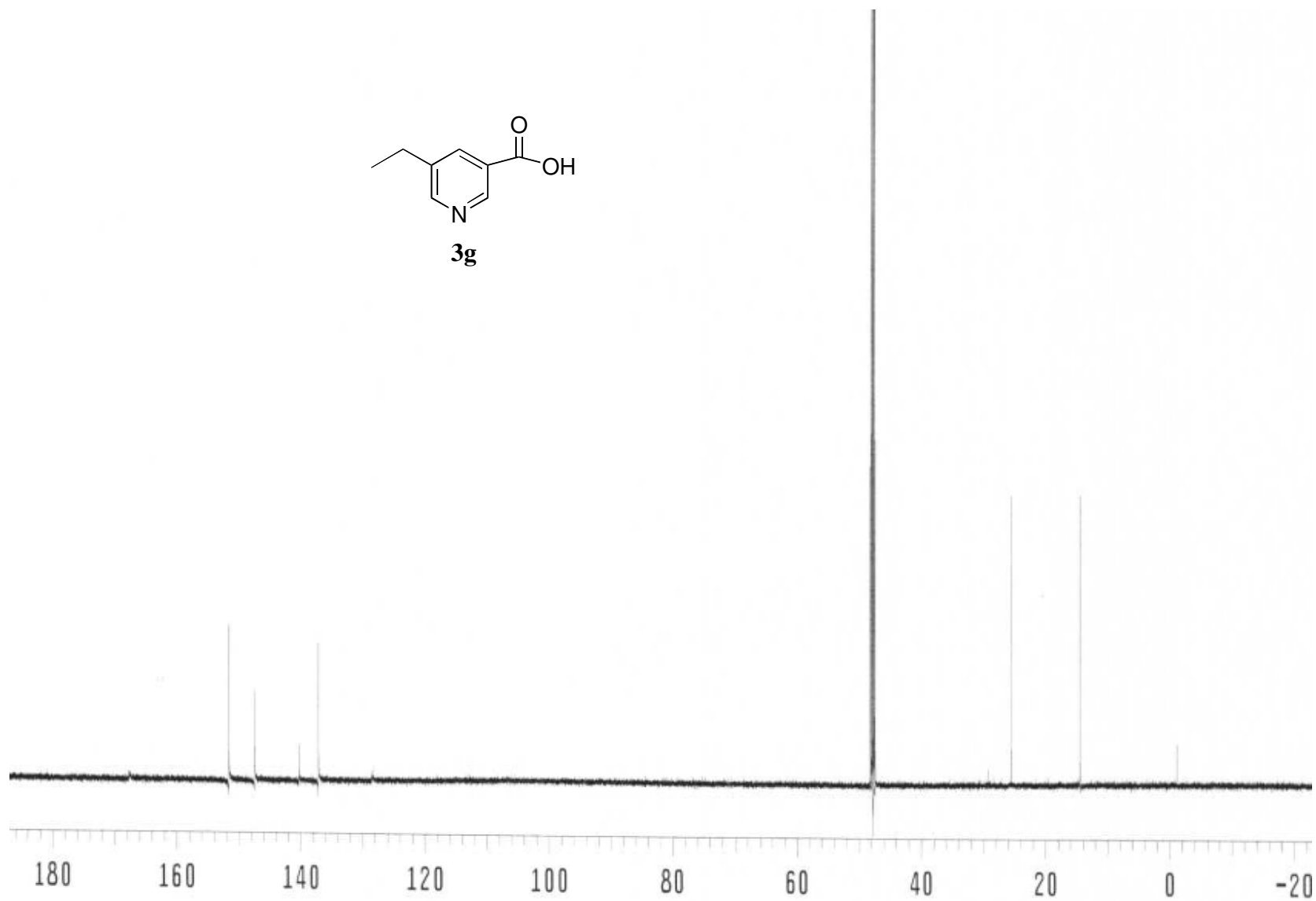
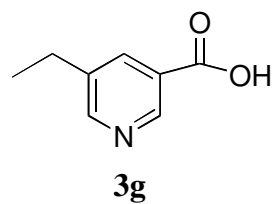
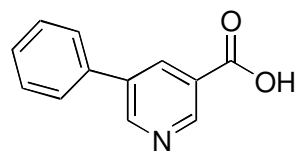


Figure S11. ¹H-NMR of **3h**: 5-phenylnicotinic acid



3h

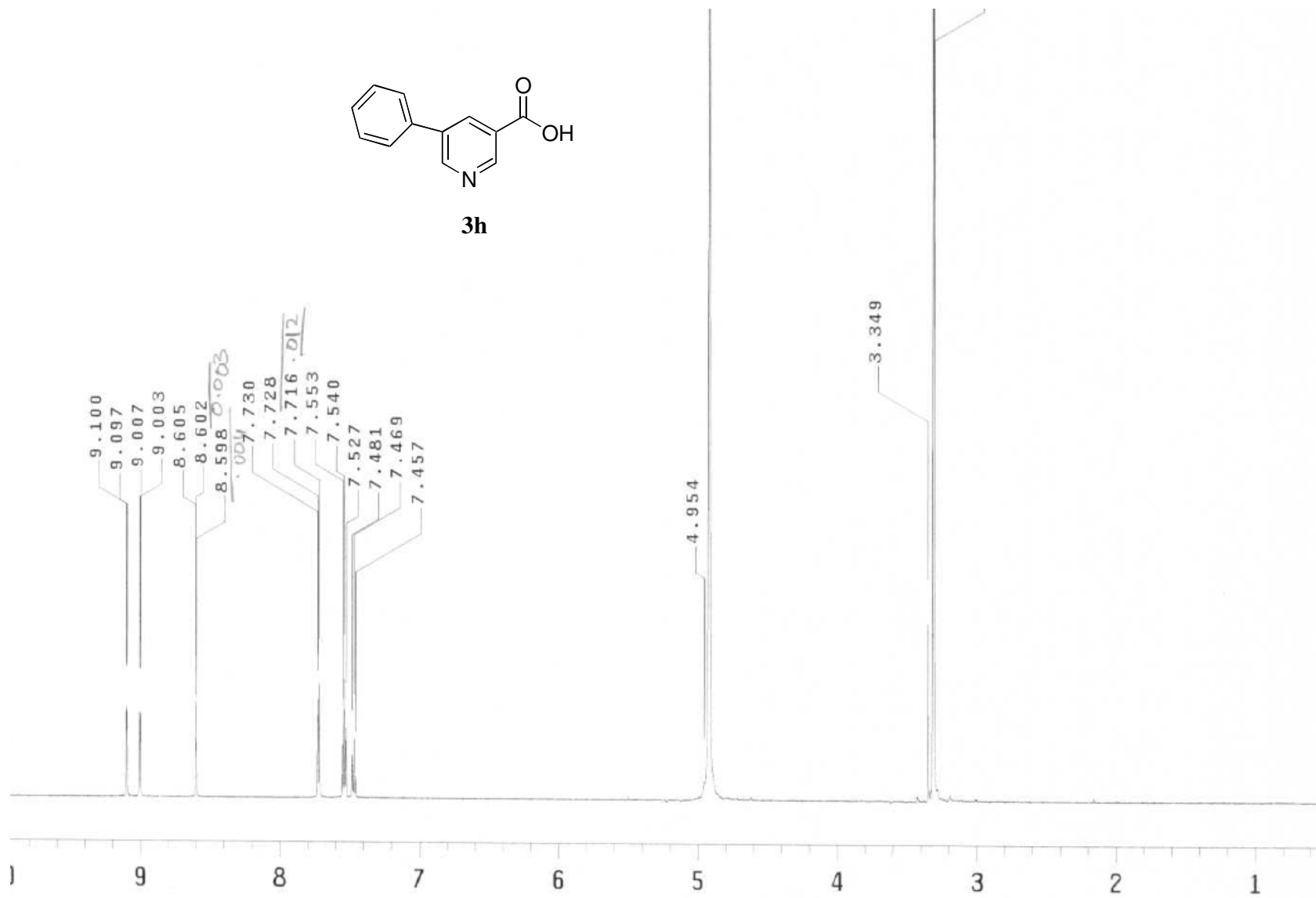


Figure S12. ^{13}C -NMR of **3h**: 5-phenylnicotinic acid

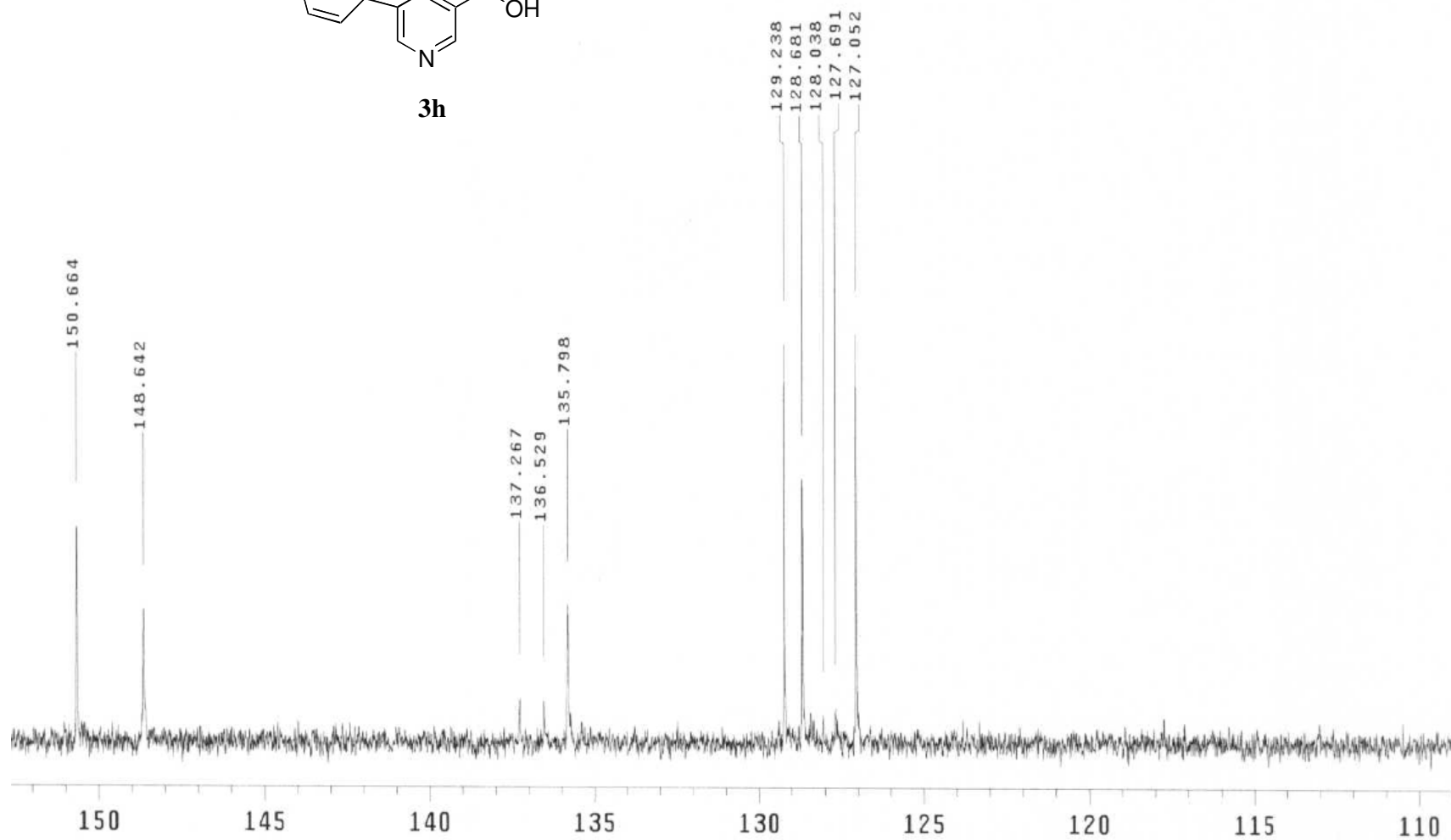
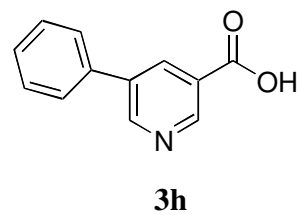


Figure S13. ¹H-NMR of **3i**: 5-azidonicotinic acid

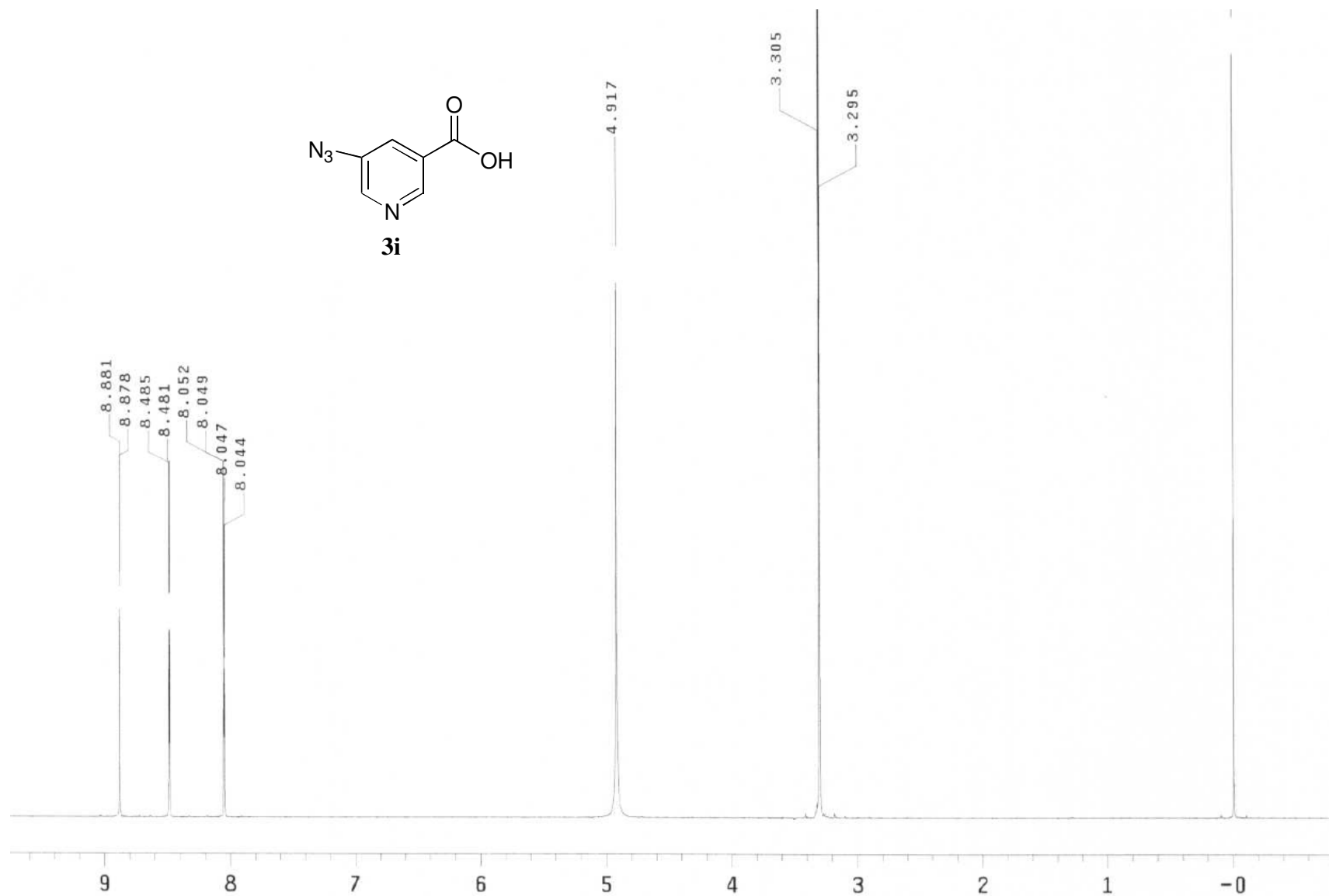


Figure S14. ^{13}C -NMR of **3i**: 5-azidonicotinic acid

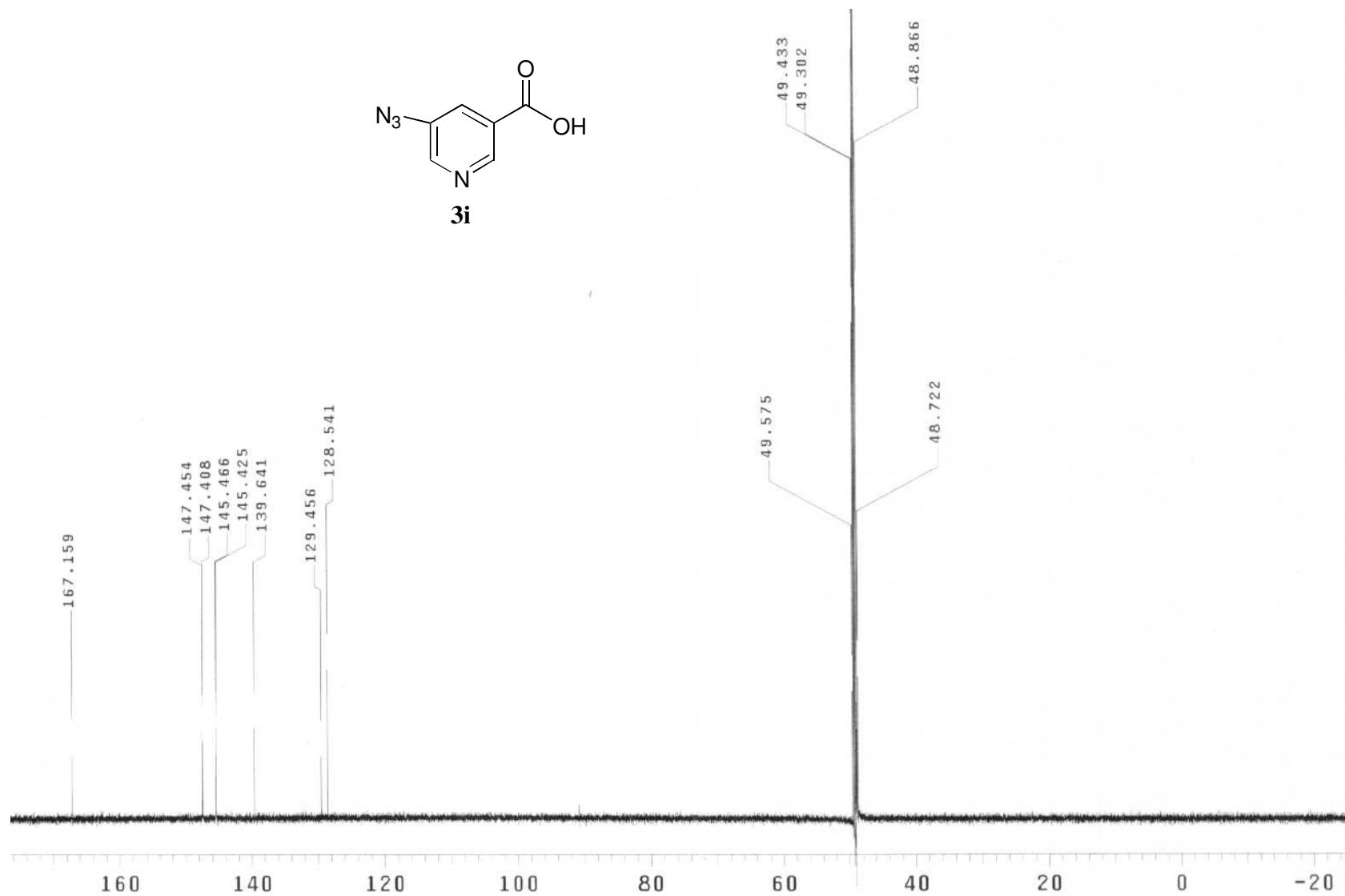


Figure S15. ¹H-NMR of **3j**: 5-(4-(aminomethyl)-1H-1,2,3,-triazol-1-yl)nicotinic acid

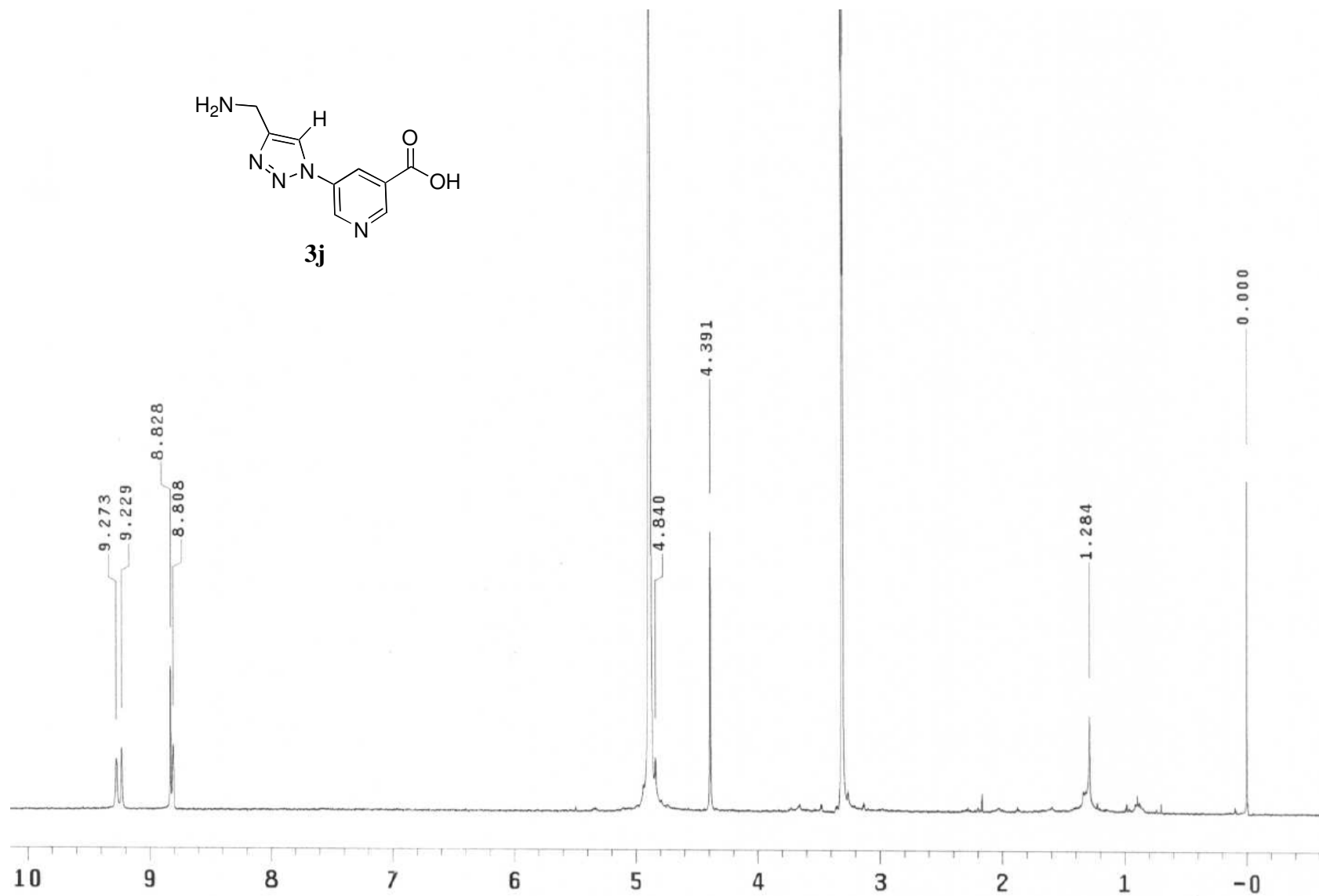


Figure S16. ¹H-NMR of **4**: 3-bromo-5-(4,5-dihydro-4,4-dimethyl-2-oxazolyl)-pyridine

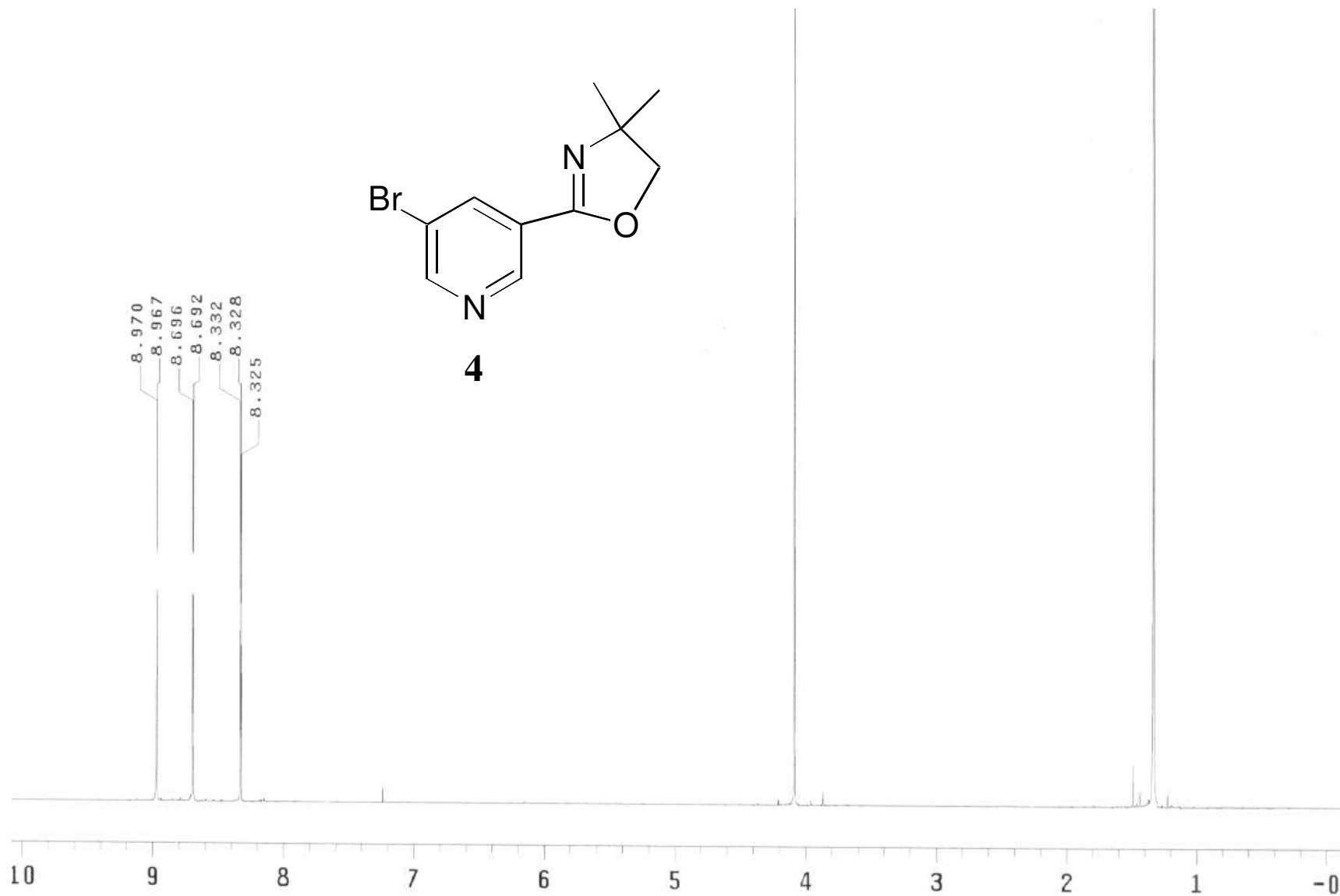


Figure S17 ¹H-NMR of **5**: 1,2-bis(5-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)-pyridin-3-yl)ethyne

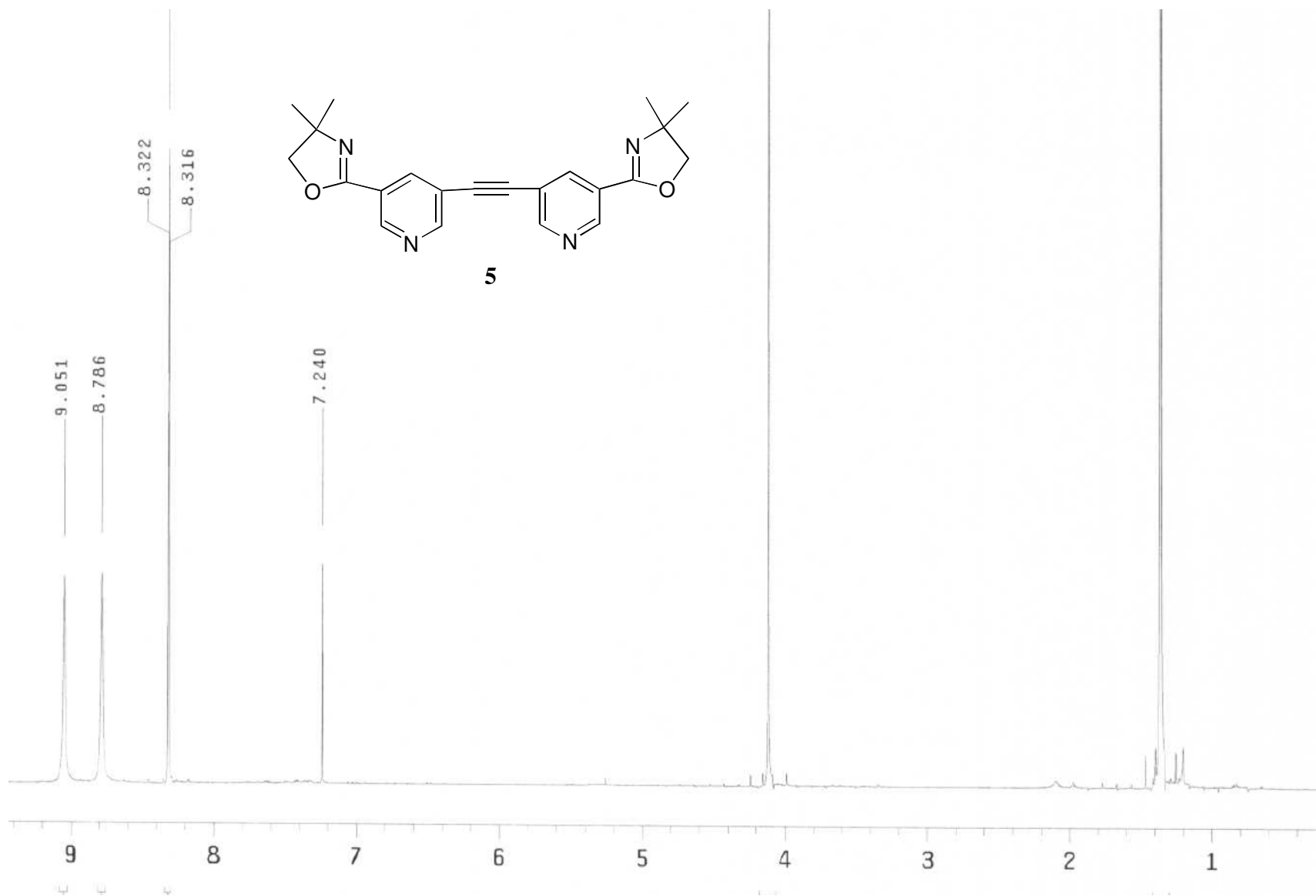


Figure S18 ¹³C-NMR of **5**: 1,2-bis(5-(4,4-dimethyl-4,5-dihydrooxazol-2-yl)-pyridin-3-yl)ethyne

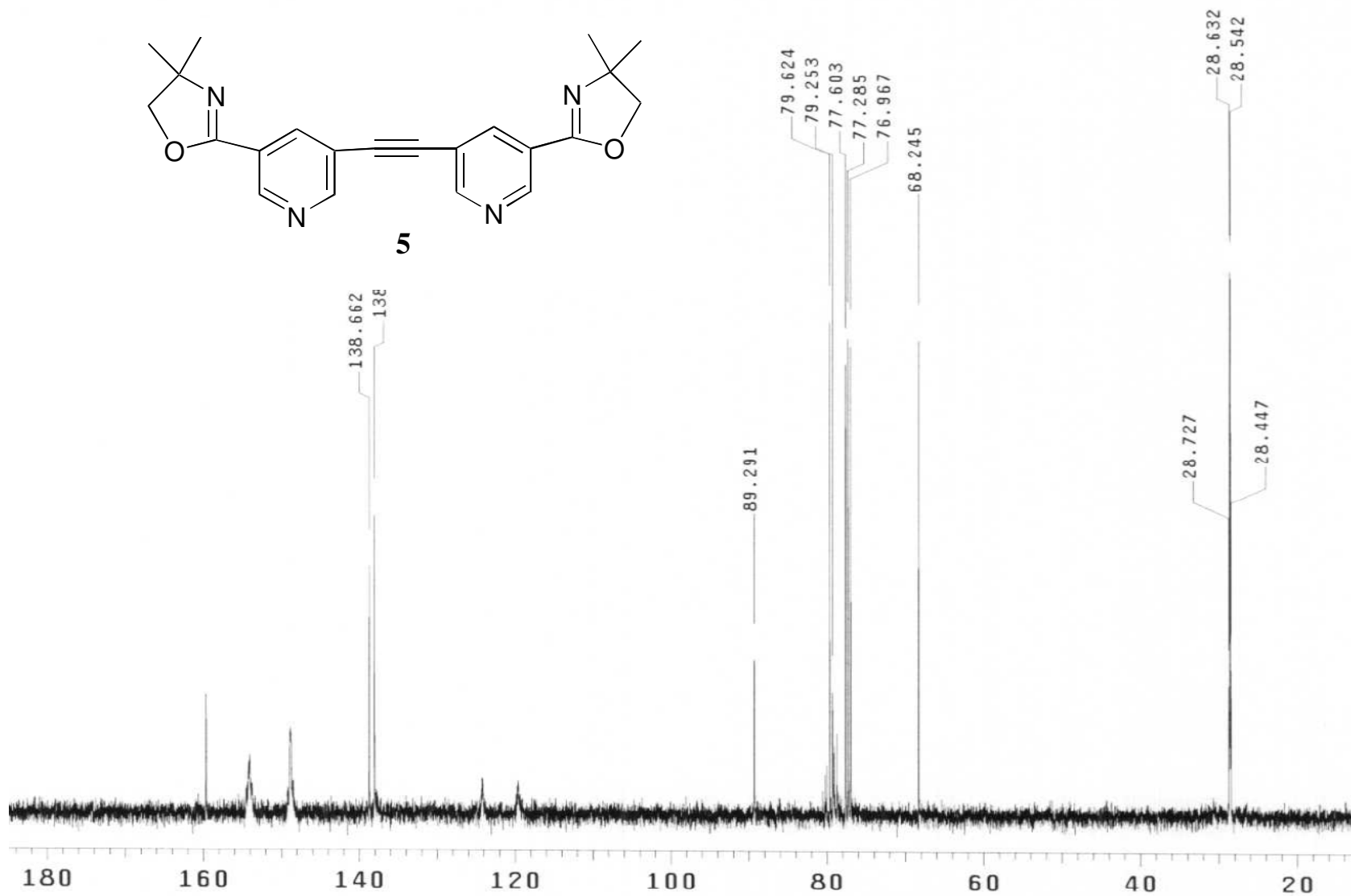


Figure S19 ¹H-NMR: 4-*n*-butyl-3-(4,5-dihydro-4,4-dimethyl-2-oxazolyl)-pyridine

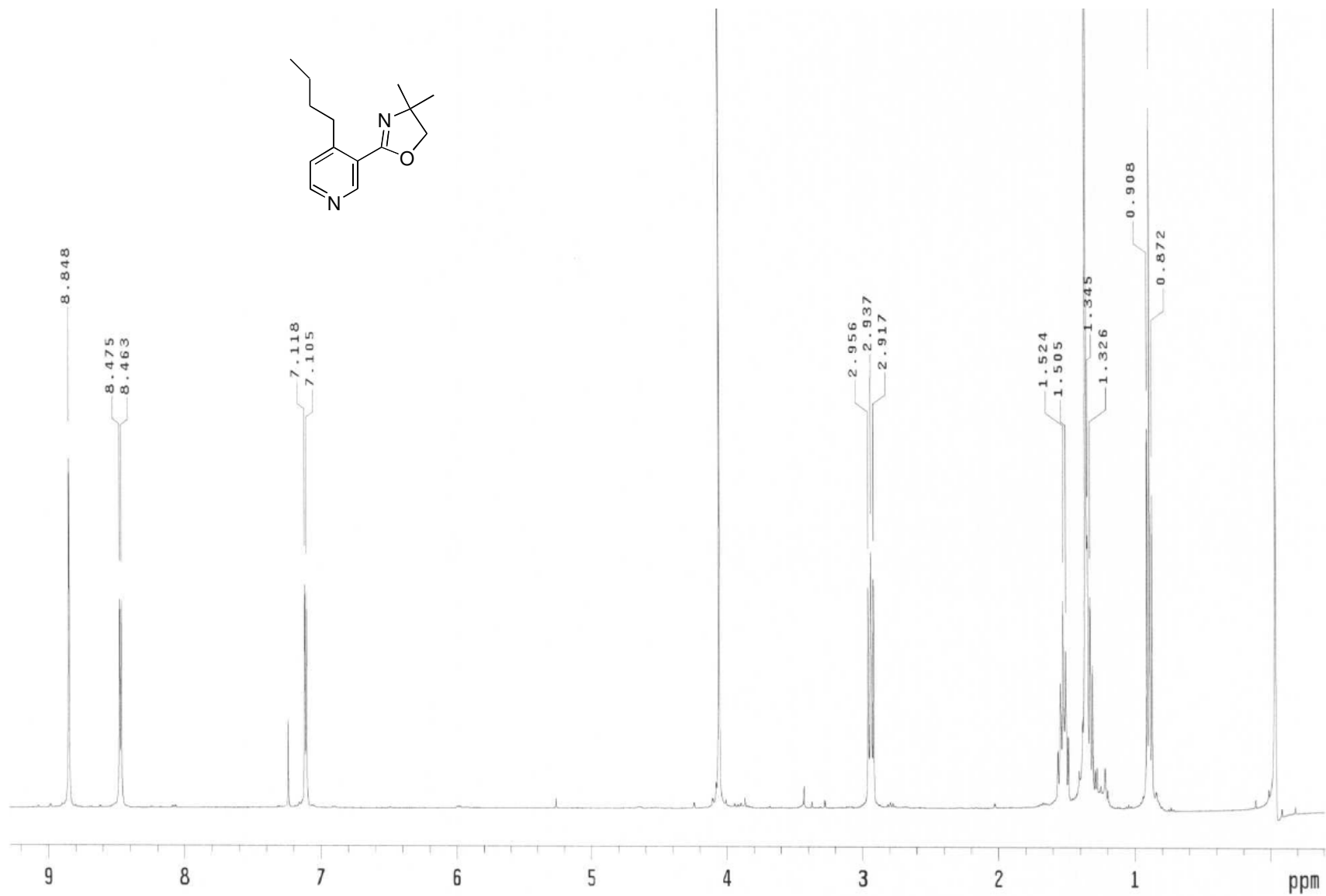


Figure S20 ¹H-NMR: 4-phenyl-3-(4,5-dihydro-4,4-dimethyl-2-oxazolyl)-pyridine

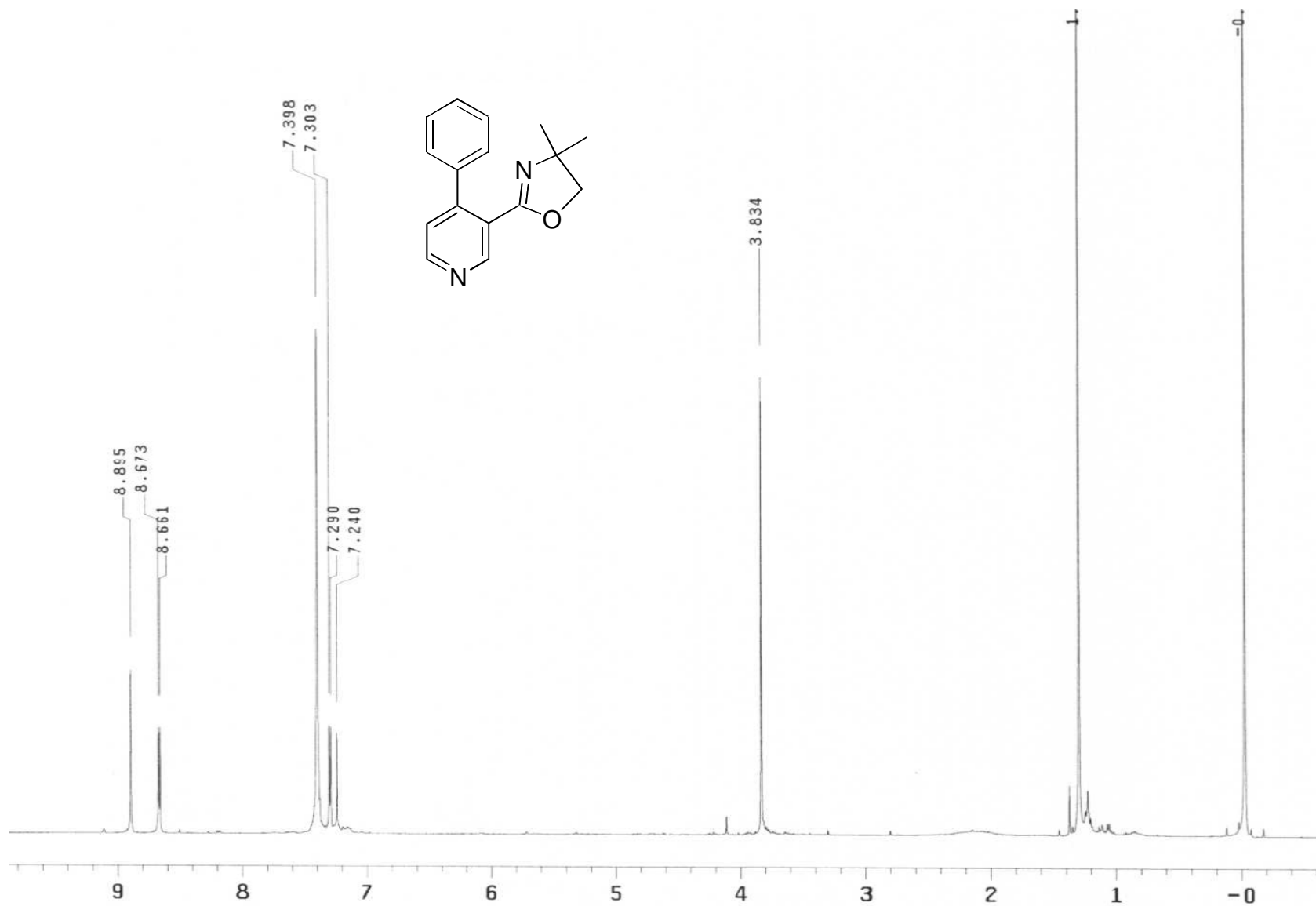


Figure S21 ¹H-NMR of **6**: 4,4-dimethyl-2-(5-((triethylsilyl)ethynyl)pyridine-3-yl)-4,5-dihydrooxazole

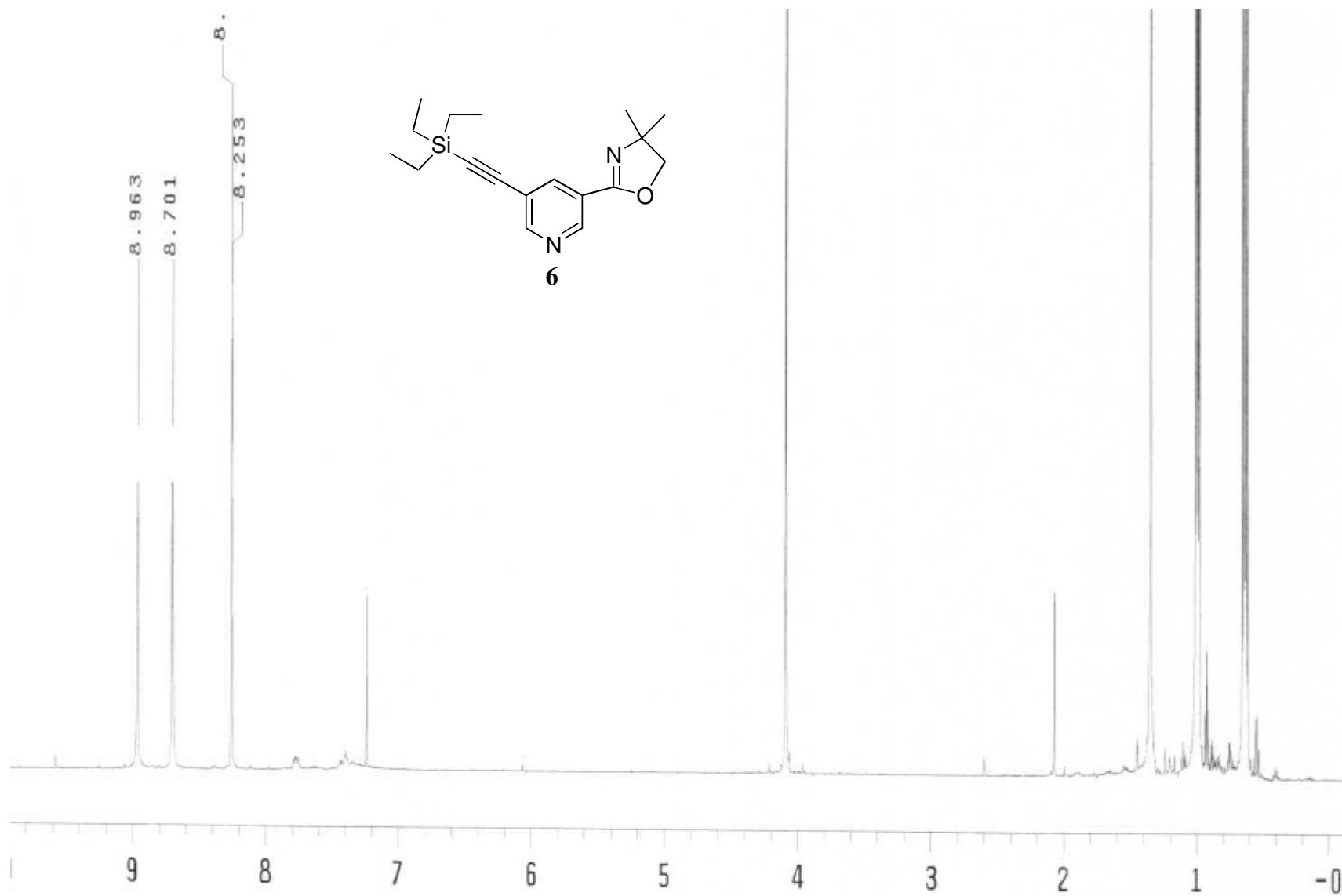


Figure S22 ^{13}C -NMR of **6**: 4,4-dimethyl-2-(5-((triethylsilyl)ethynyl)pyridine-3-yl)-4,5-dihydrooxazole

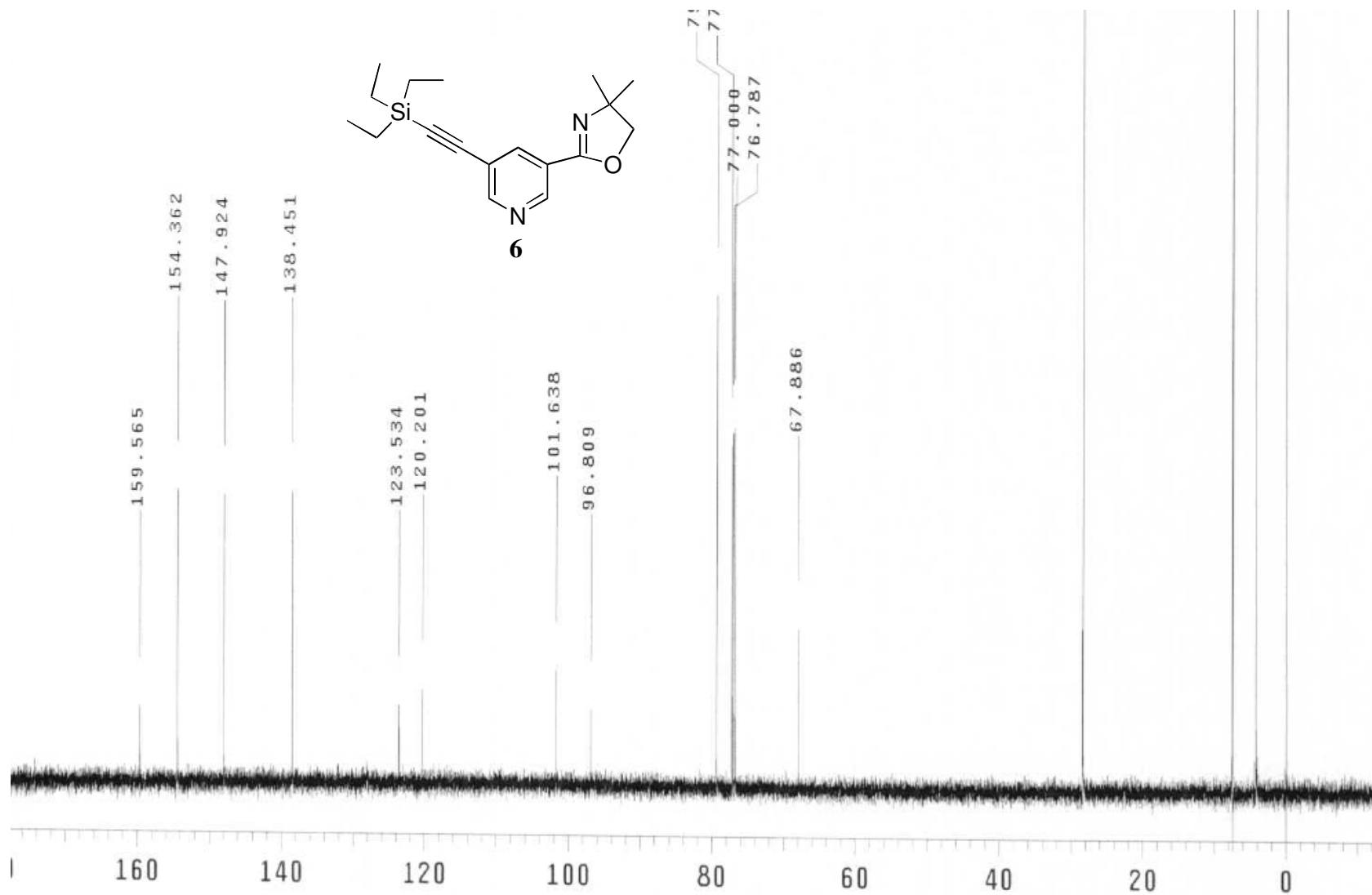


Figure S23 $^1\text{H-NMR}$: 5-ethynyl-3-(4,5-dihydro-4,4-dimethyl-2-oxazolyl)-pyridine; precursor of 5-ethylnicotinic acid (**3e**).

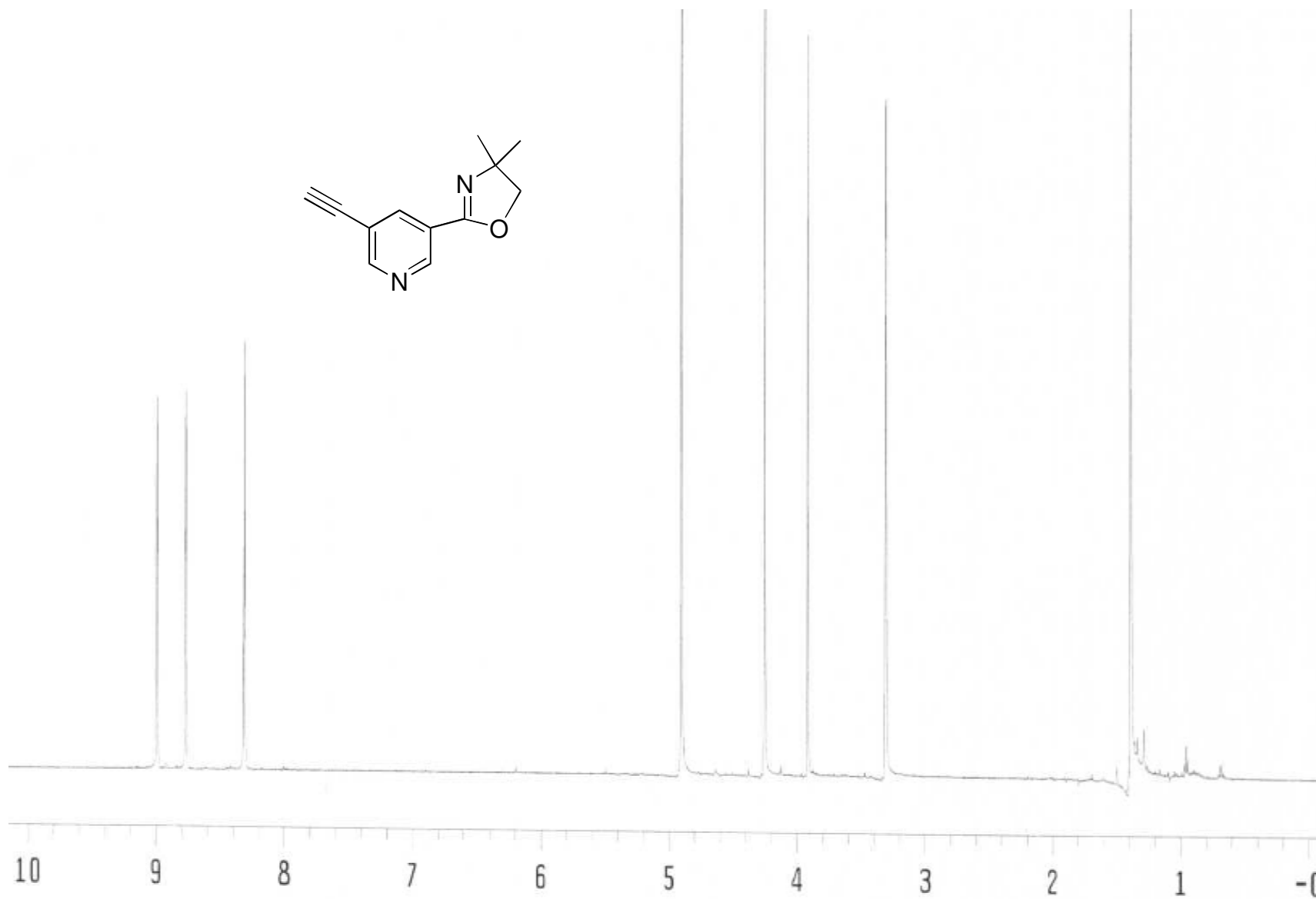


Figure S24 ^{13}C -NMR: 5-ethynyl-3-(4,5-dihydro-4,4-dimethyl-2-oxazolyl)-pyridine; precursor of 5-ethynlnicotinic acid (**3e**).

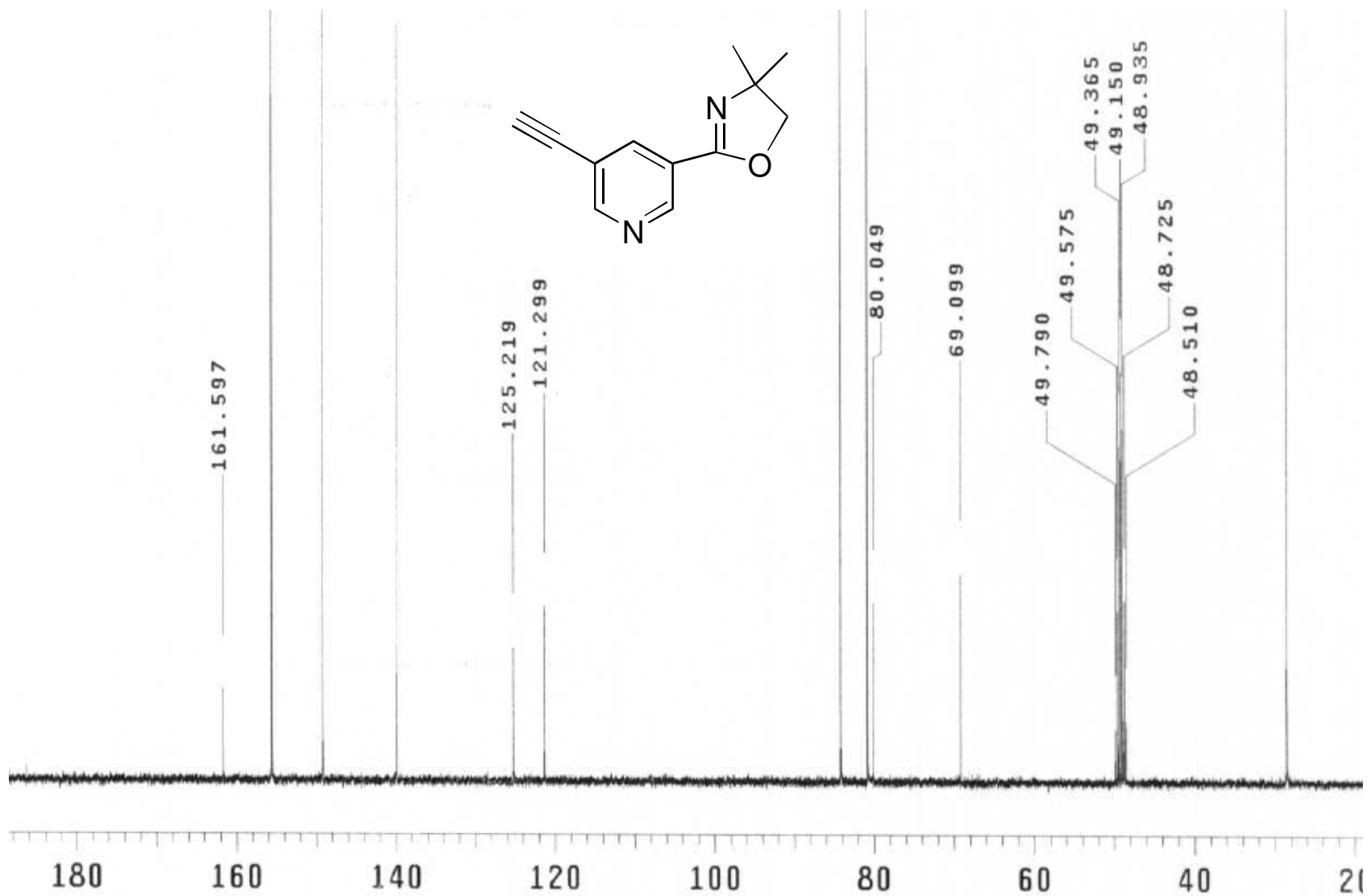


Figure S25 ¹H-NMR of **8**: pinacol ester of 5-(4,5-dihydro-4,4-dimethyl-2-oxazolyl)-3-pyridinyl boronic acid (pinacol ester **8**)

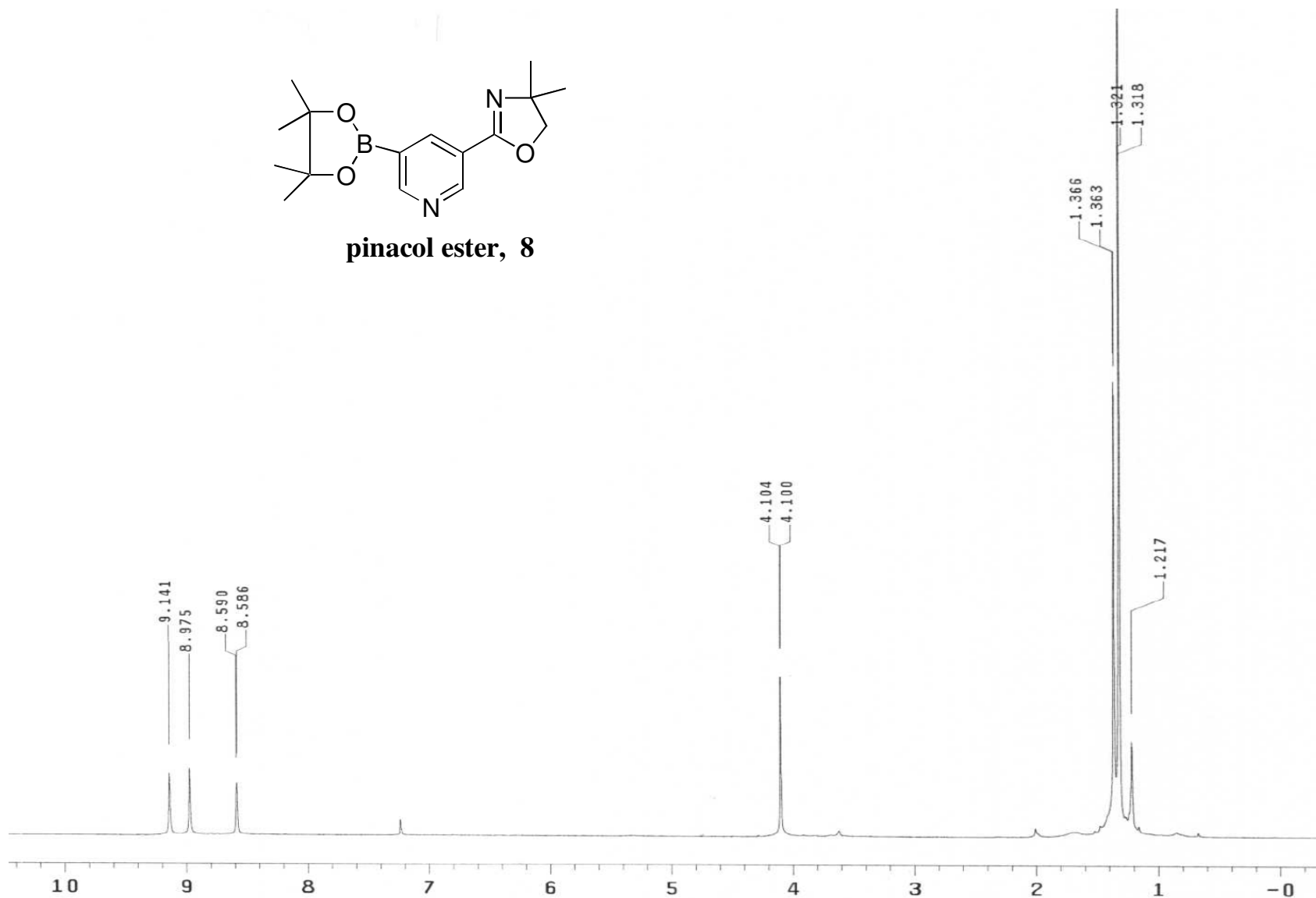


Figure S26 $^1\text{H-NMR}$ of **9**: 5-phenyl-3-(4,5-dihydro-4,4-dimethyl-2-oxazolyl)-pyridine

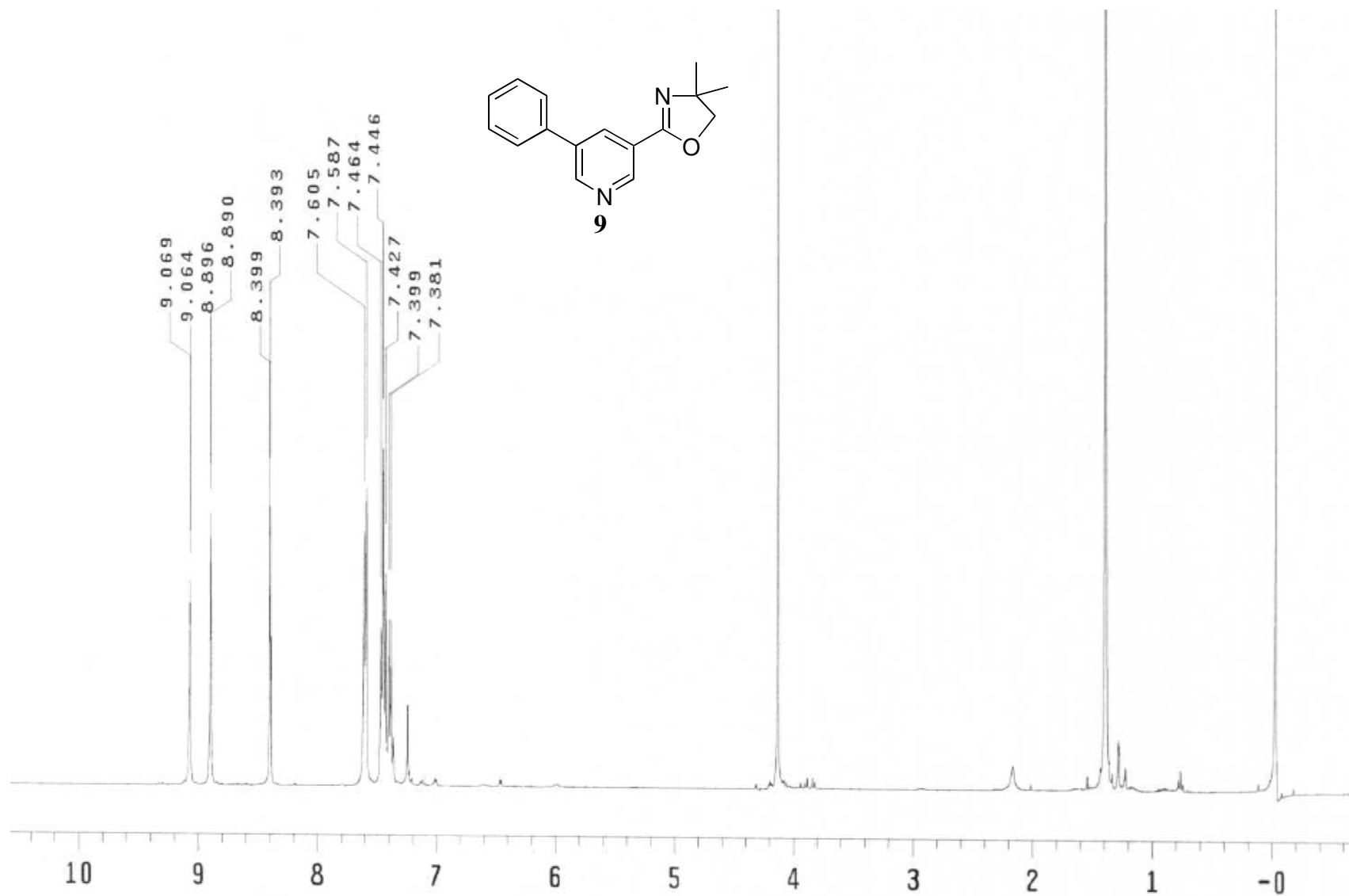


Figure S27 ^{13}C -NMR of **9**: 5-phenyl-3-(4,5-dihydro-4,4-dimethyl-2-oxazolyl)-pyridine

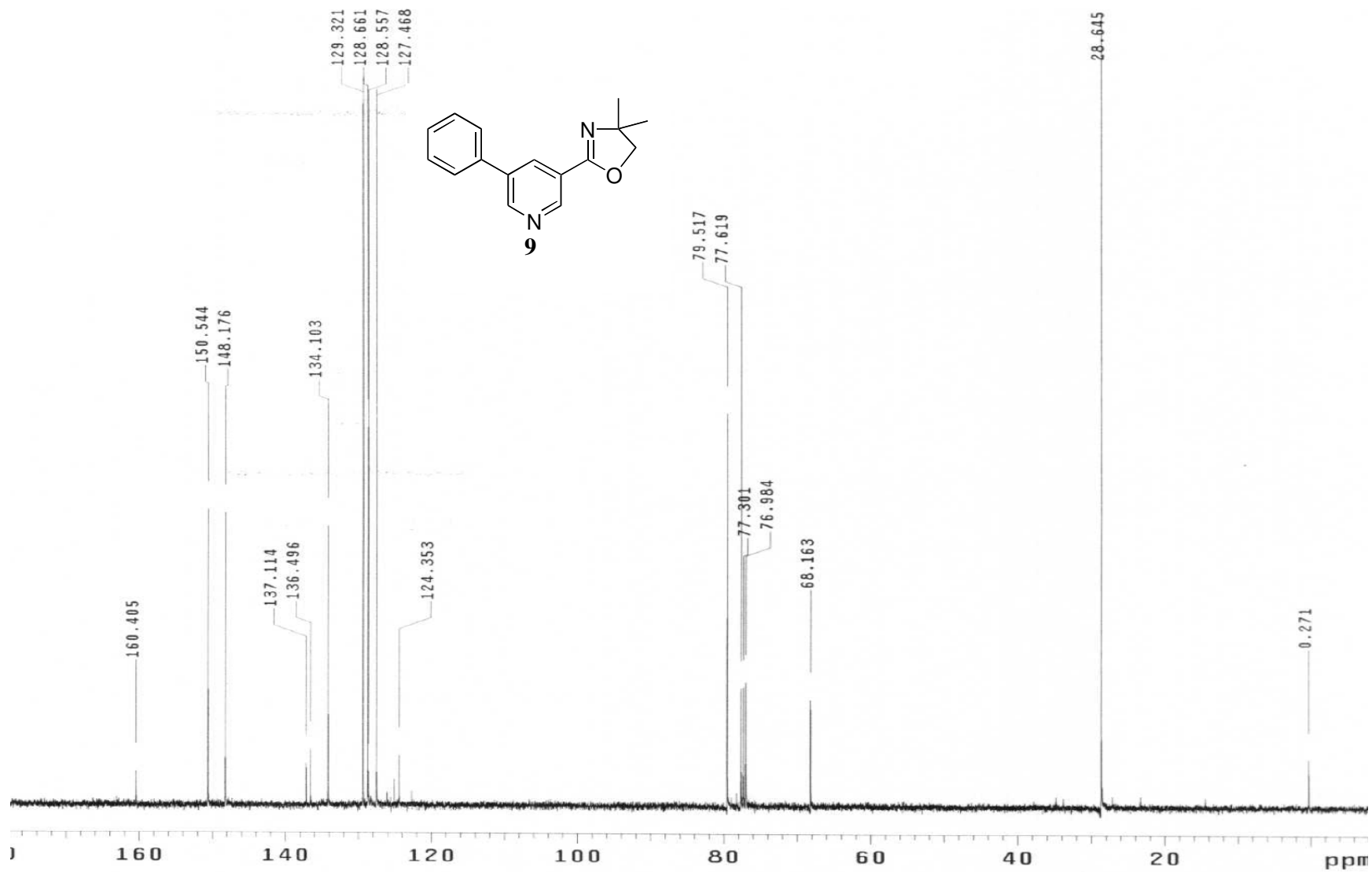


Figure S28 $^1\text{H-NMR}$ of **10**: 5-aminonicotinic acid ethyl ester

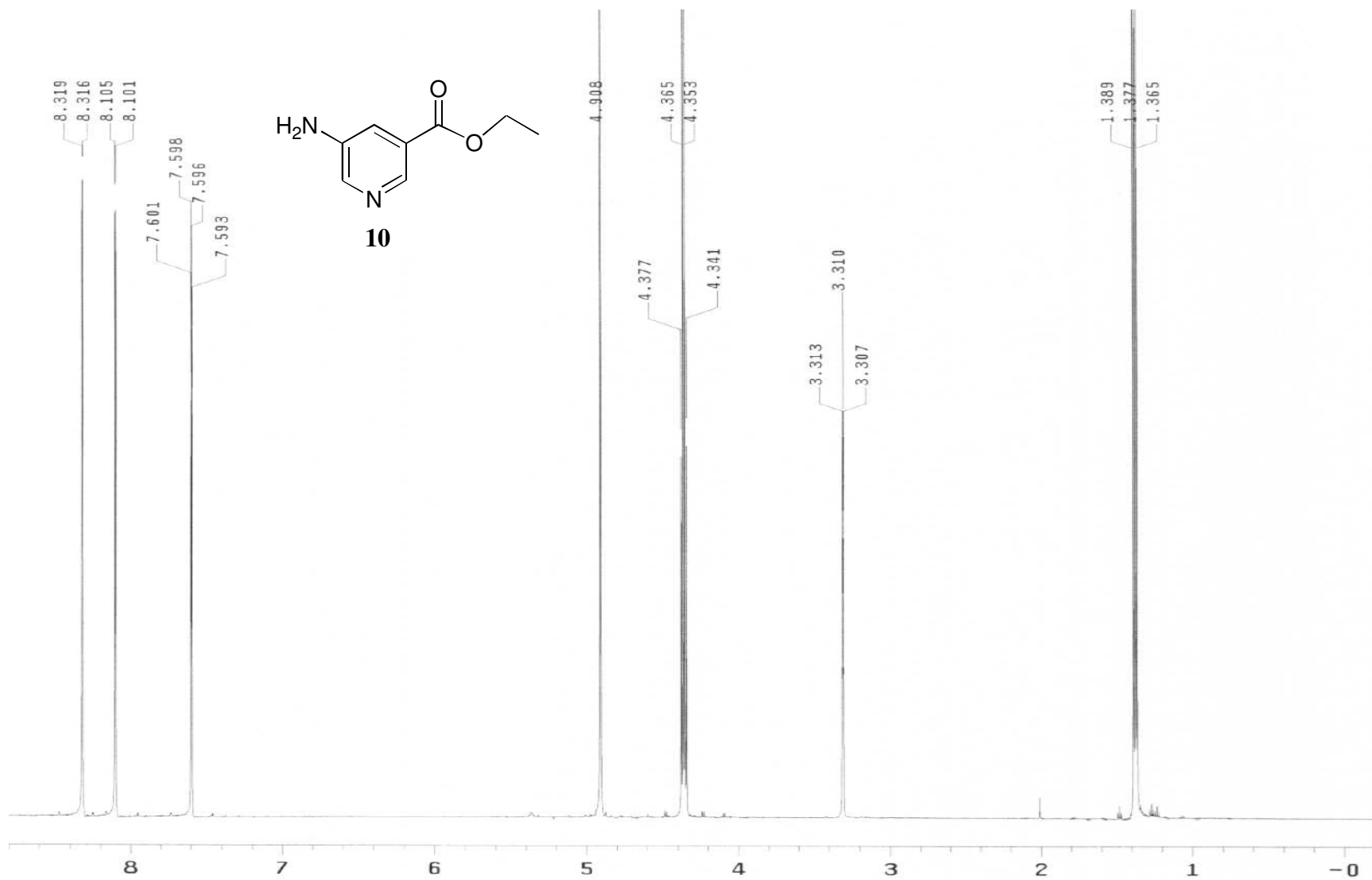


Figure S29 ^{13}C -NMR of **10**: 5-aminonicotinic acid ethyl ester

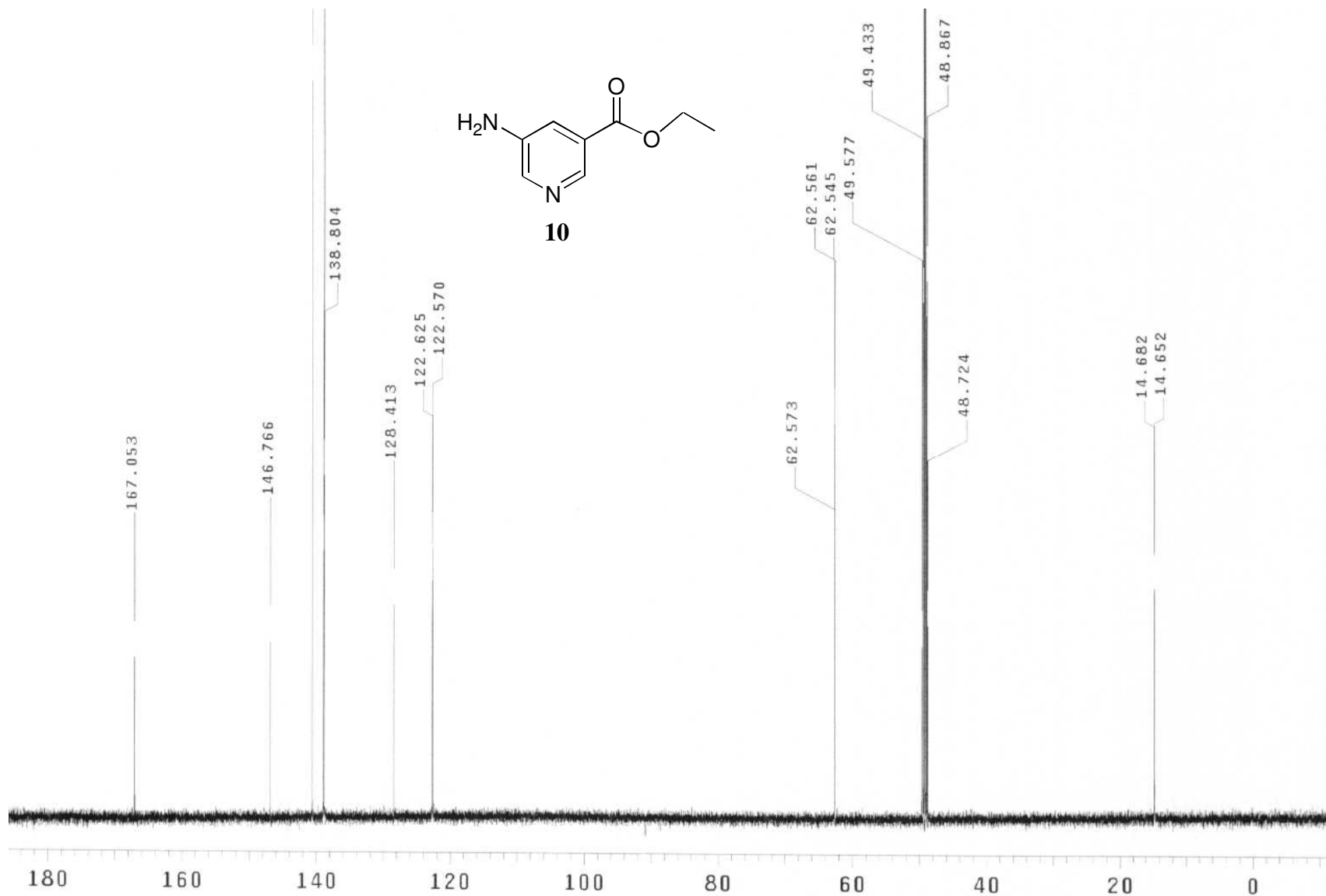


Figure S30 ¹H-NMR of **11**: 5-azidonicotinic acid ethyl ester

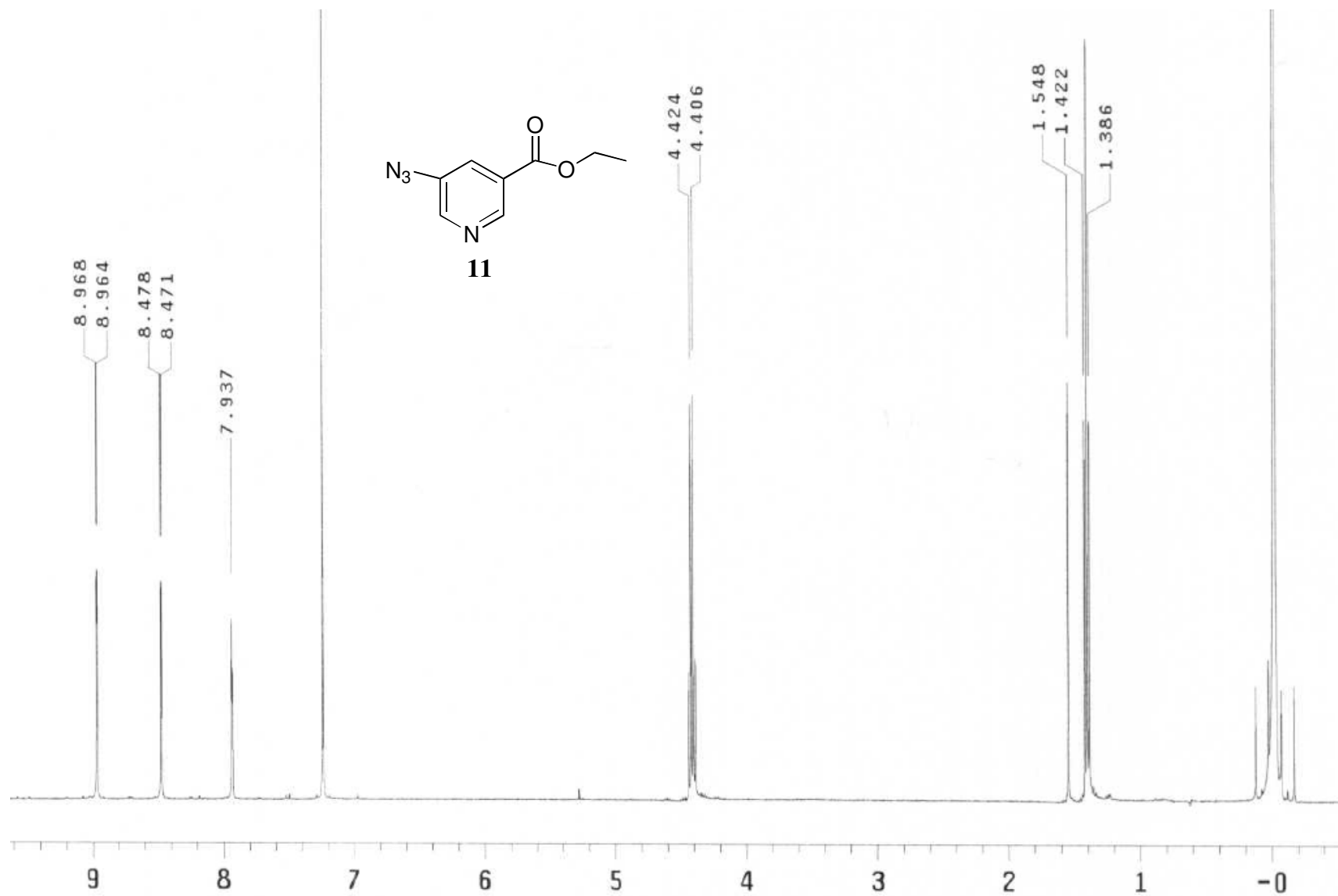


Figure S31 ^{13}C -NMR of **11**: 5-azidonicotinic acid ethyl ester

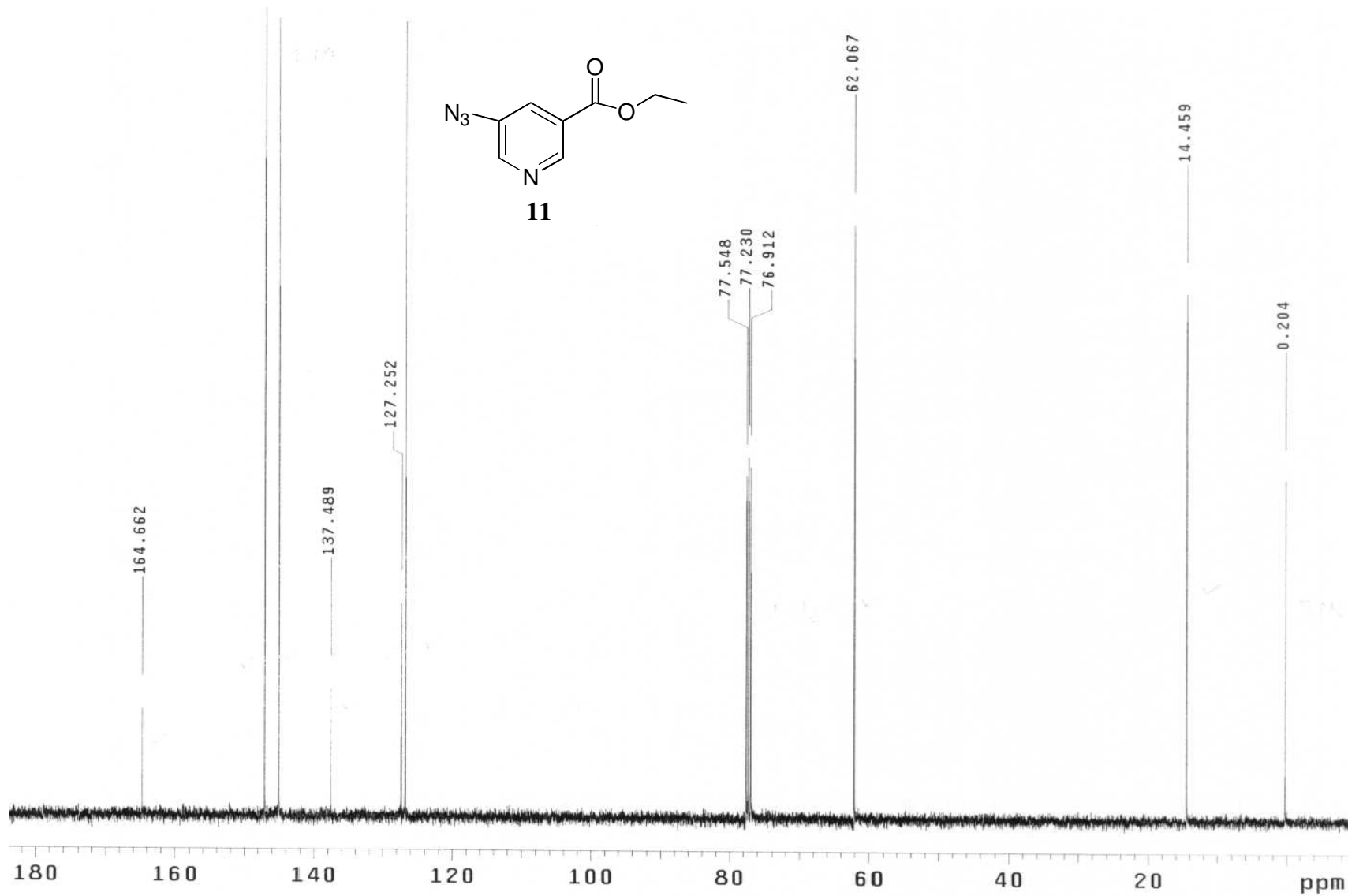


Figure S32 ¹H-NMR of **14**: ethyl 5-(4-(aminomethyl)-1*H*-1,2,3-triazol-1-yl)nicotinate

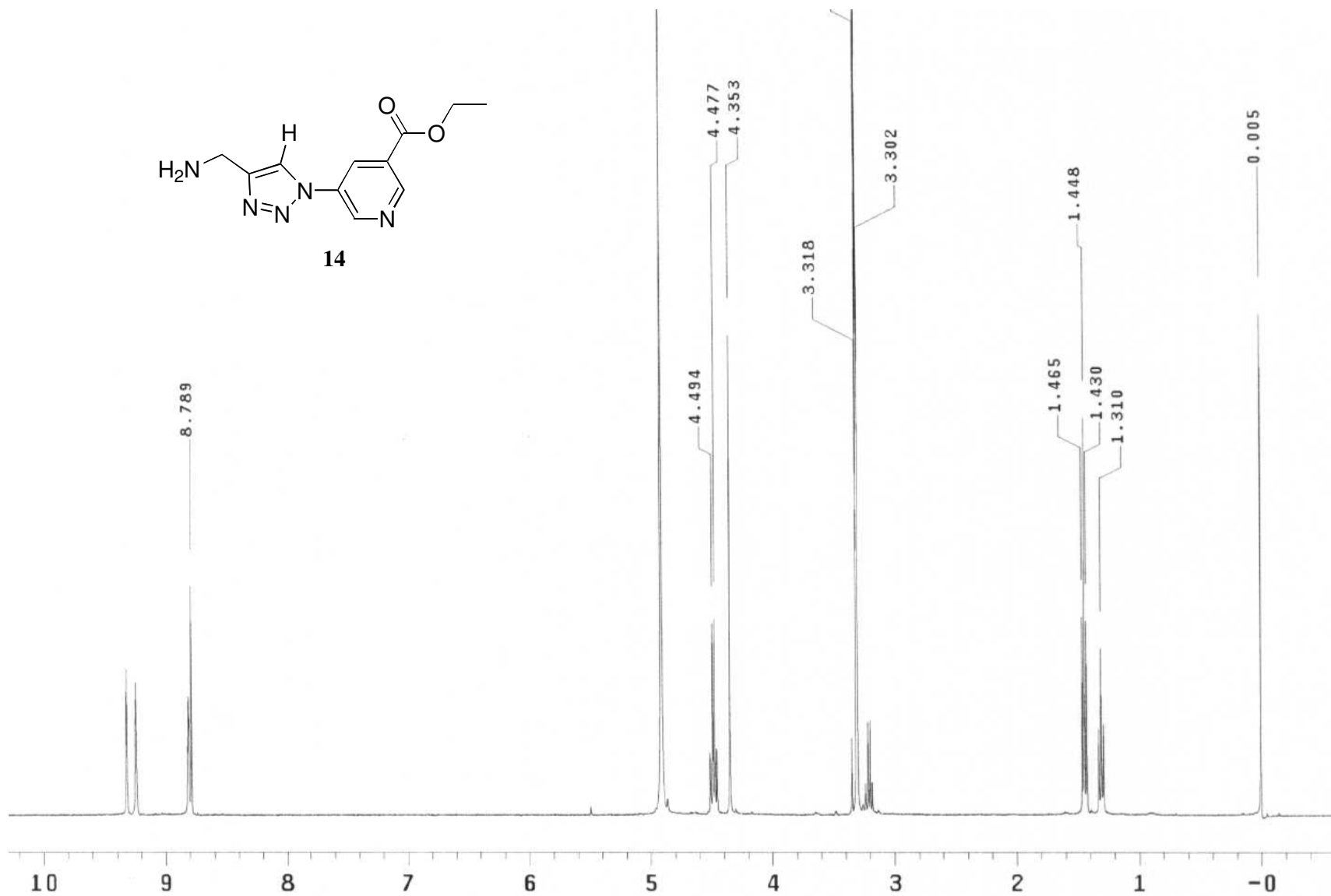


Figure S33 ^{13}C -NMR of **14**: ethyl 5-(4-(aminomethyl)-1*H*-1,2,3-triazol-1-yl)nicotinate

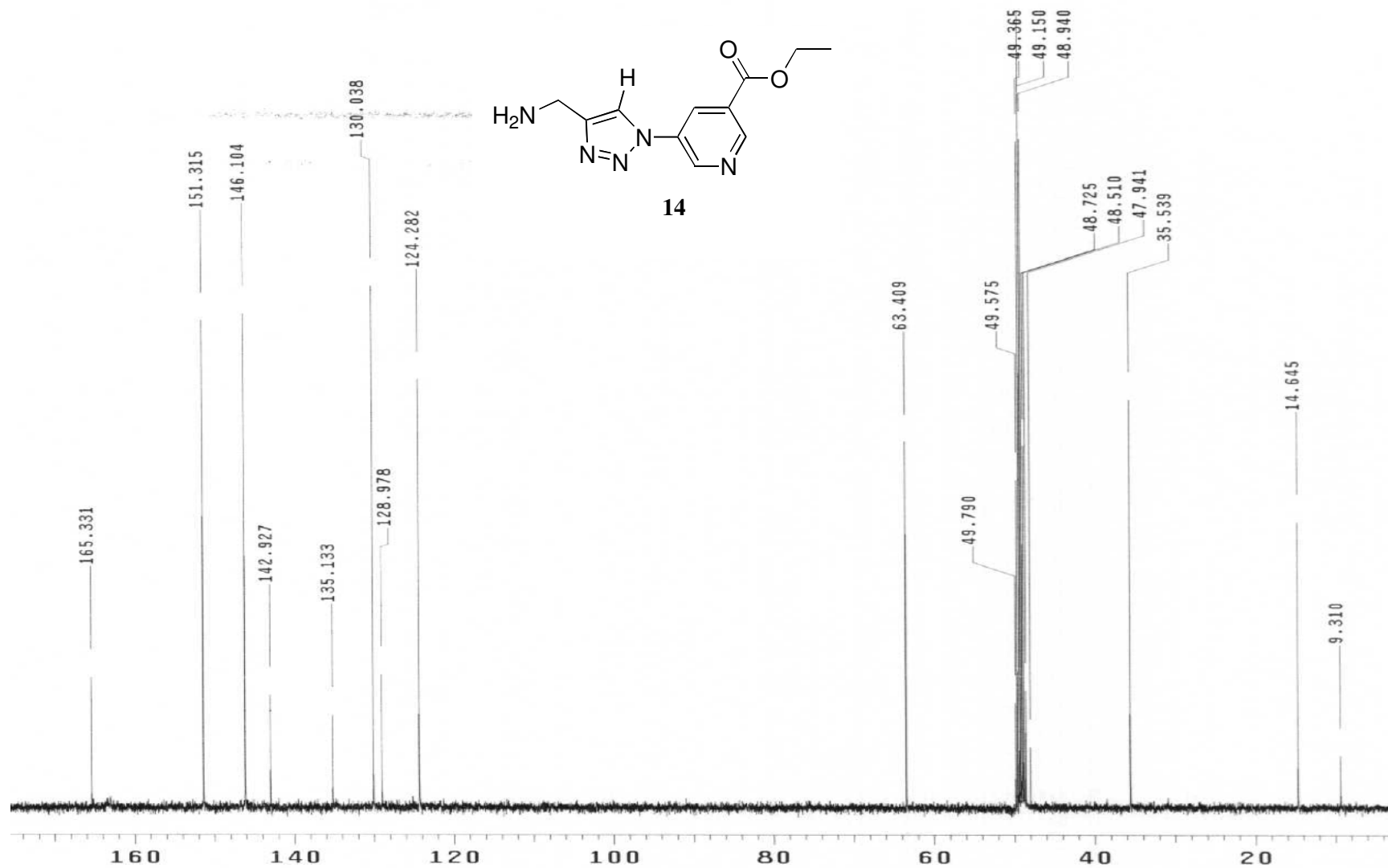


Figure S34 ¹H-NMR: 4-aminonicotinic acid methyl ester

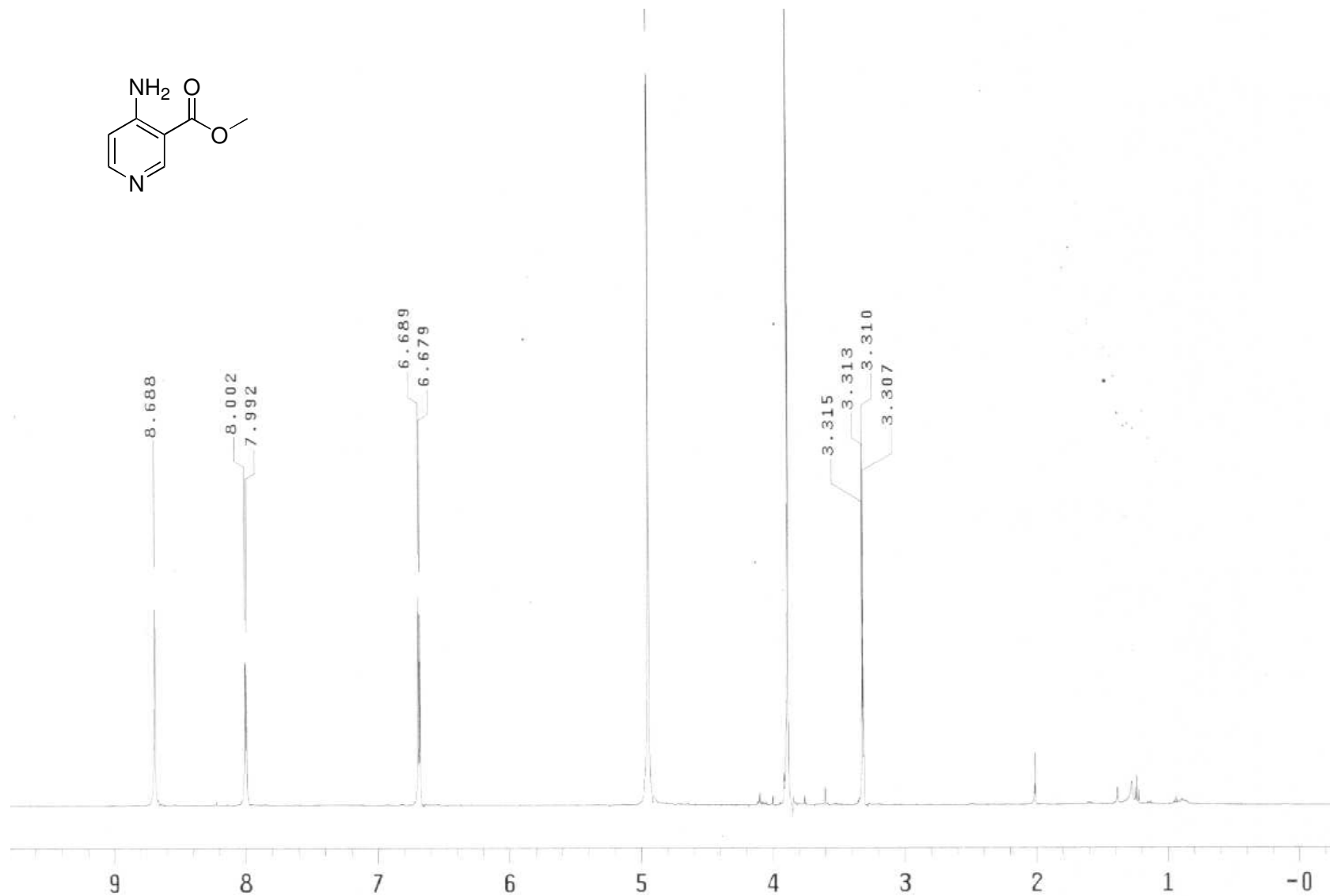


Figure S35 ^{13}C -NMR: 4-aminonicotinic acid methyl ester

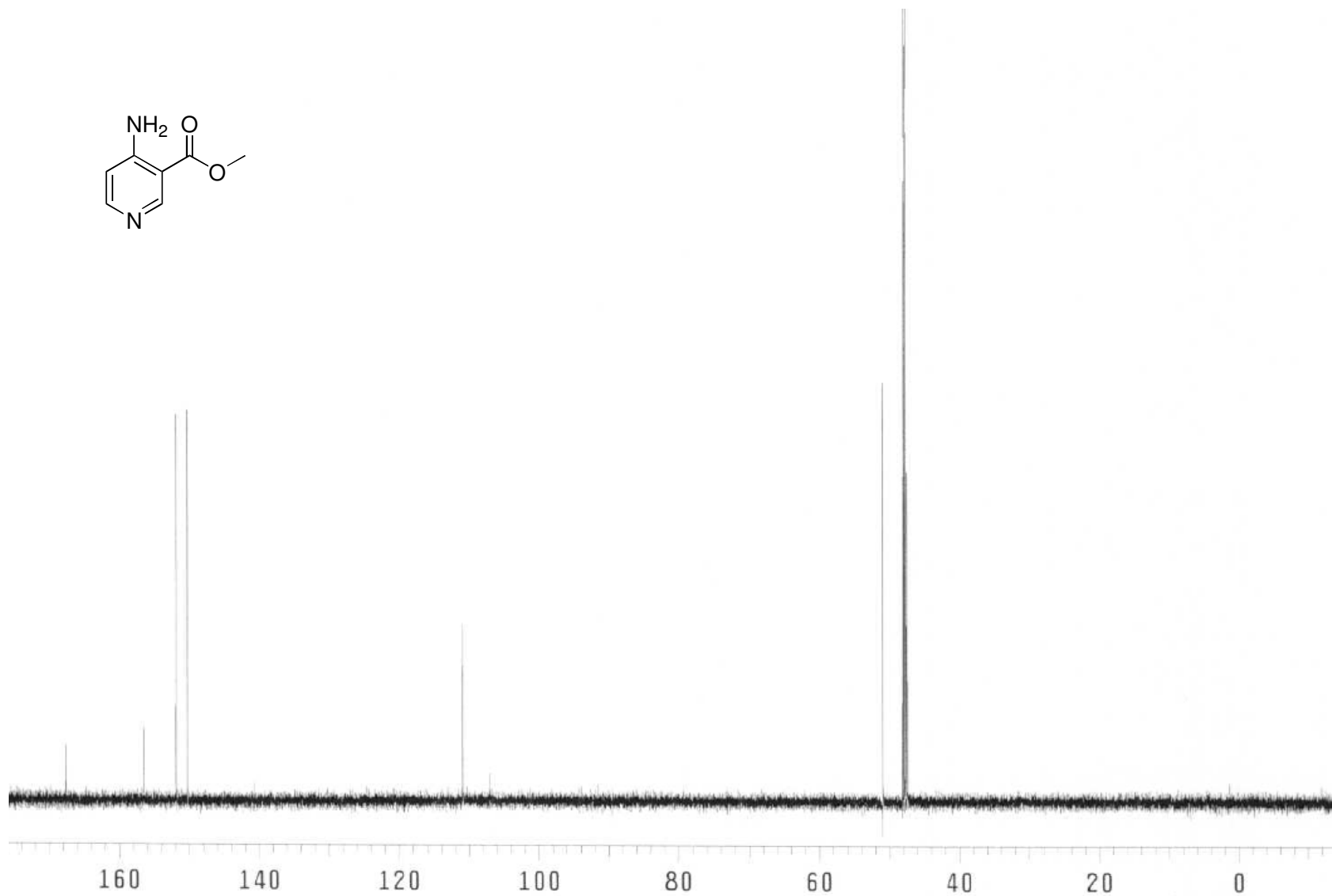
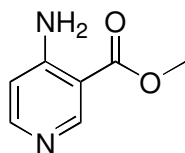


Figure S36. ¹H-NMR of **15**: 4-aminonicotinic acid methyl ester adenine dinucleotide phosphate

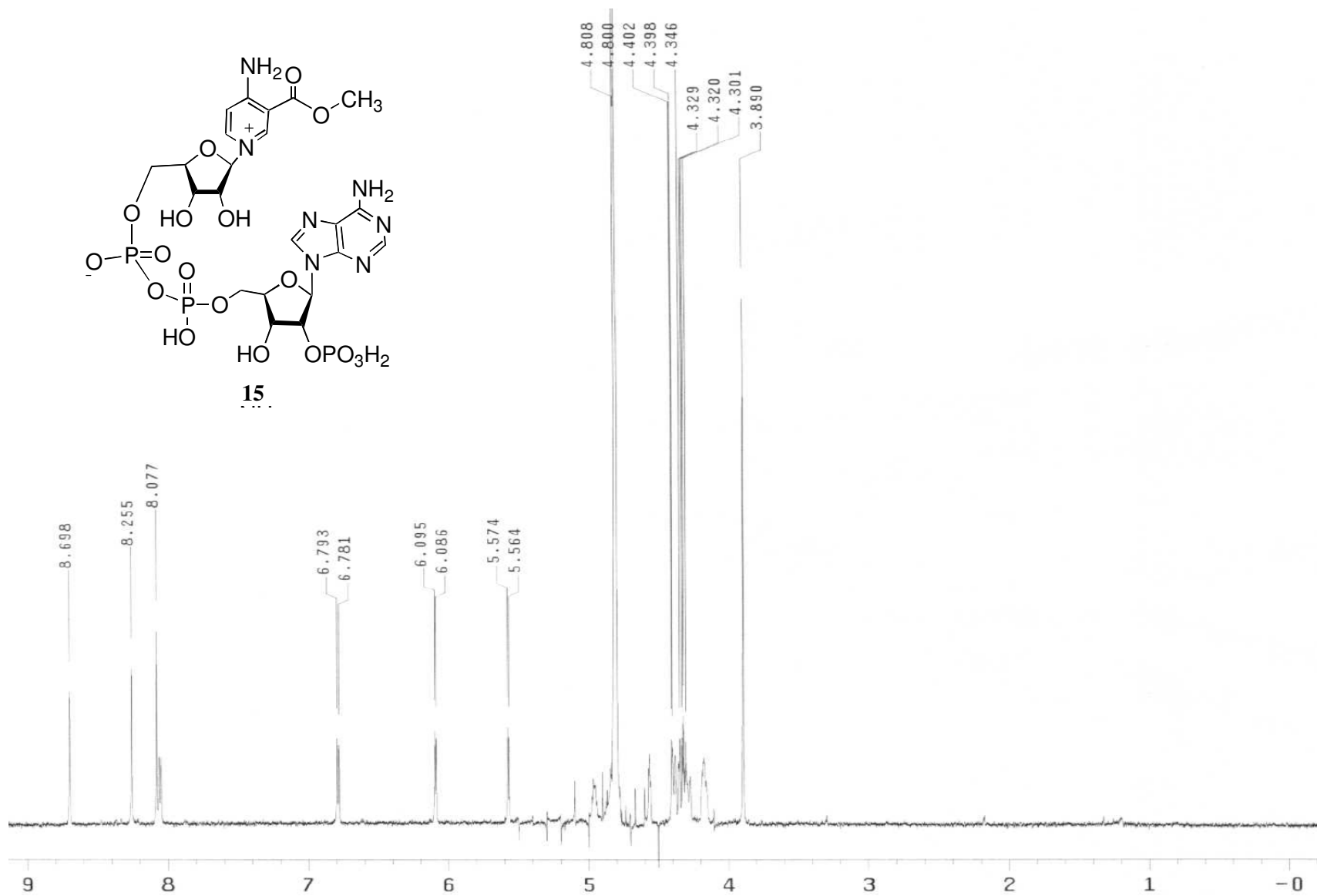


Figure S37. ^{31}P -NMR of **2c**: 4-aminonicotinic acid methyl ester adenine dinucleotide phosphate

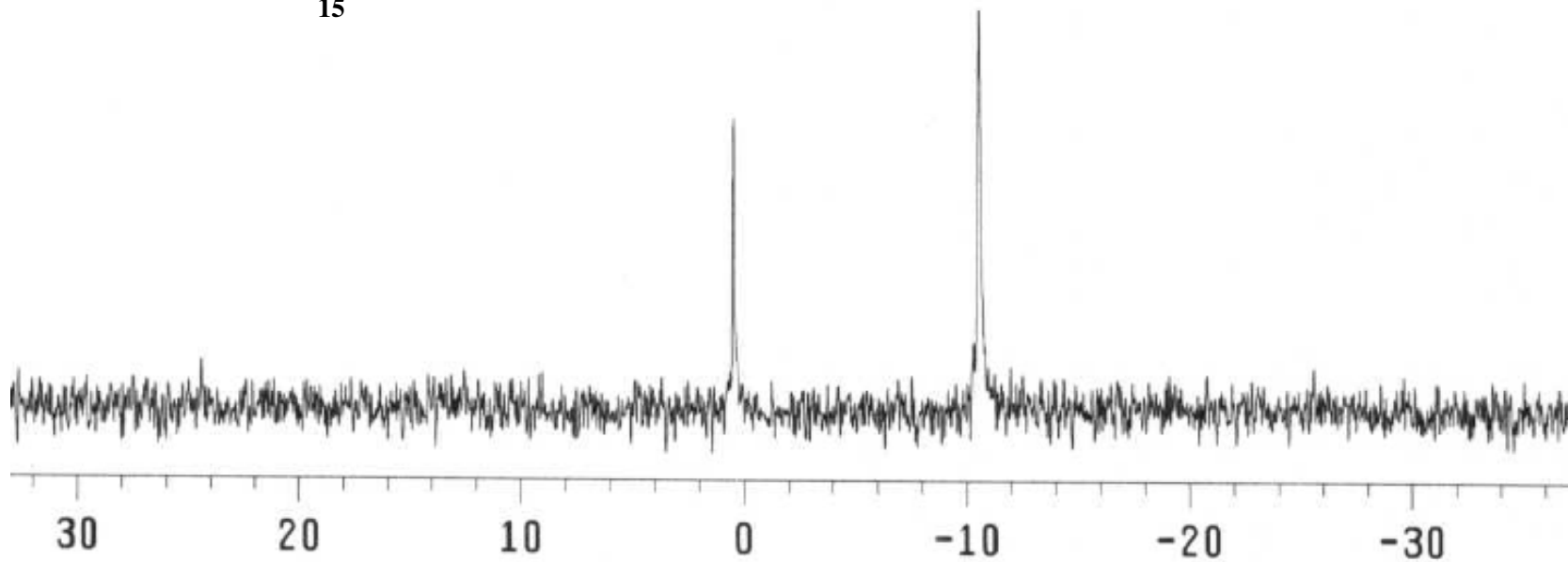
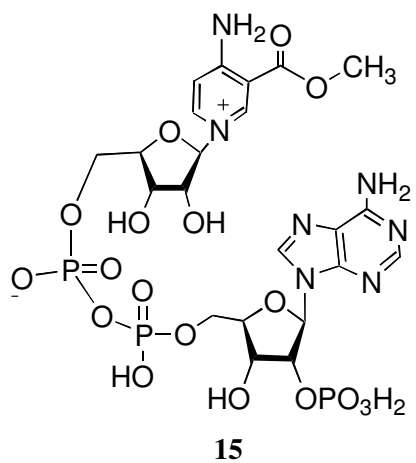


Figure S38. $^1\text{H-NMR}$ of **16**: 4-amino-NAADP

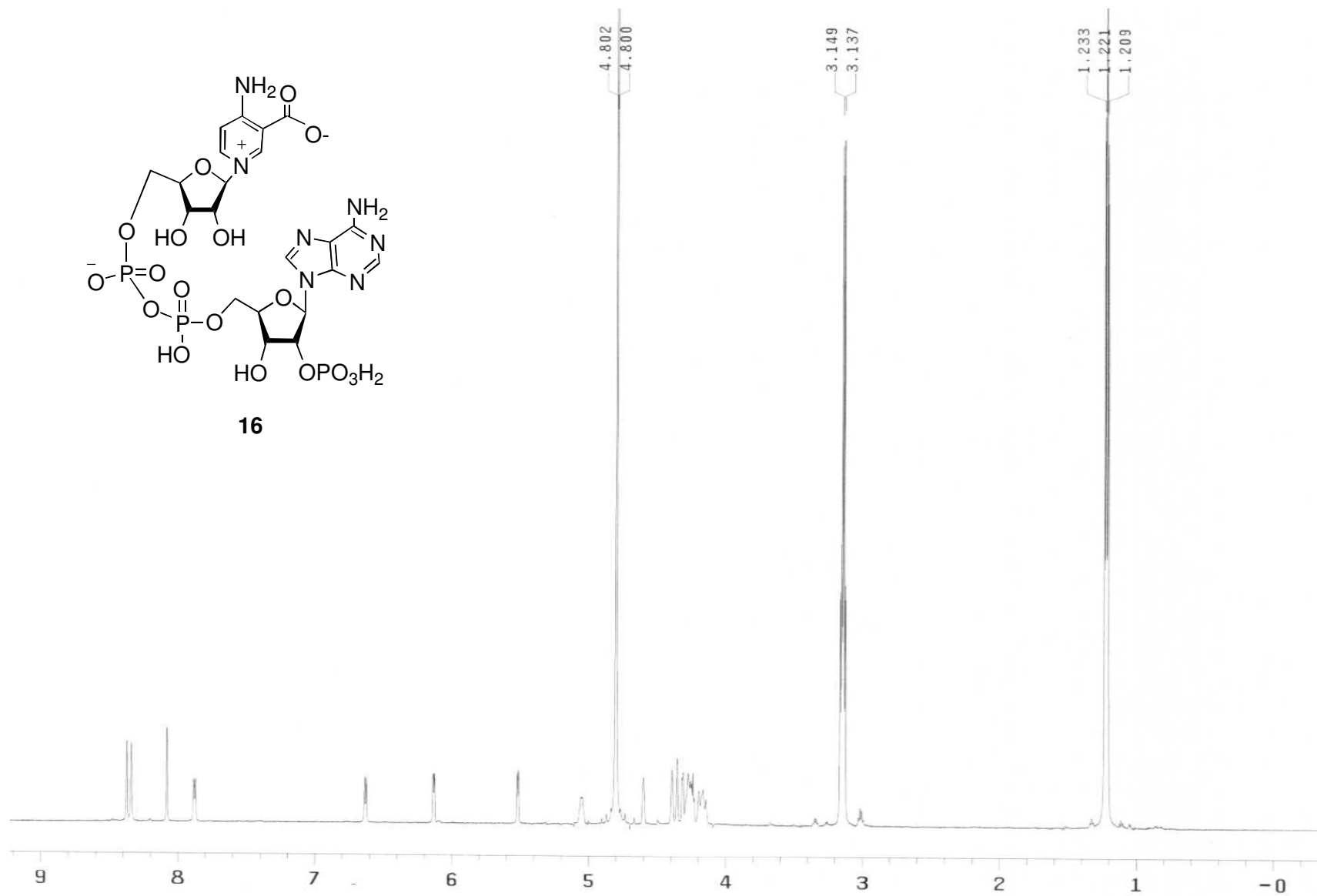


Figure S39. ^{31}P -NMR of **16**: 4-amino-NAADP

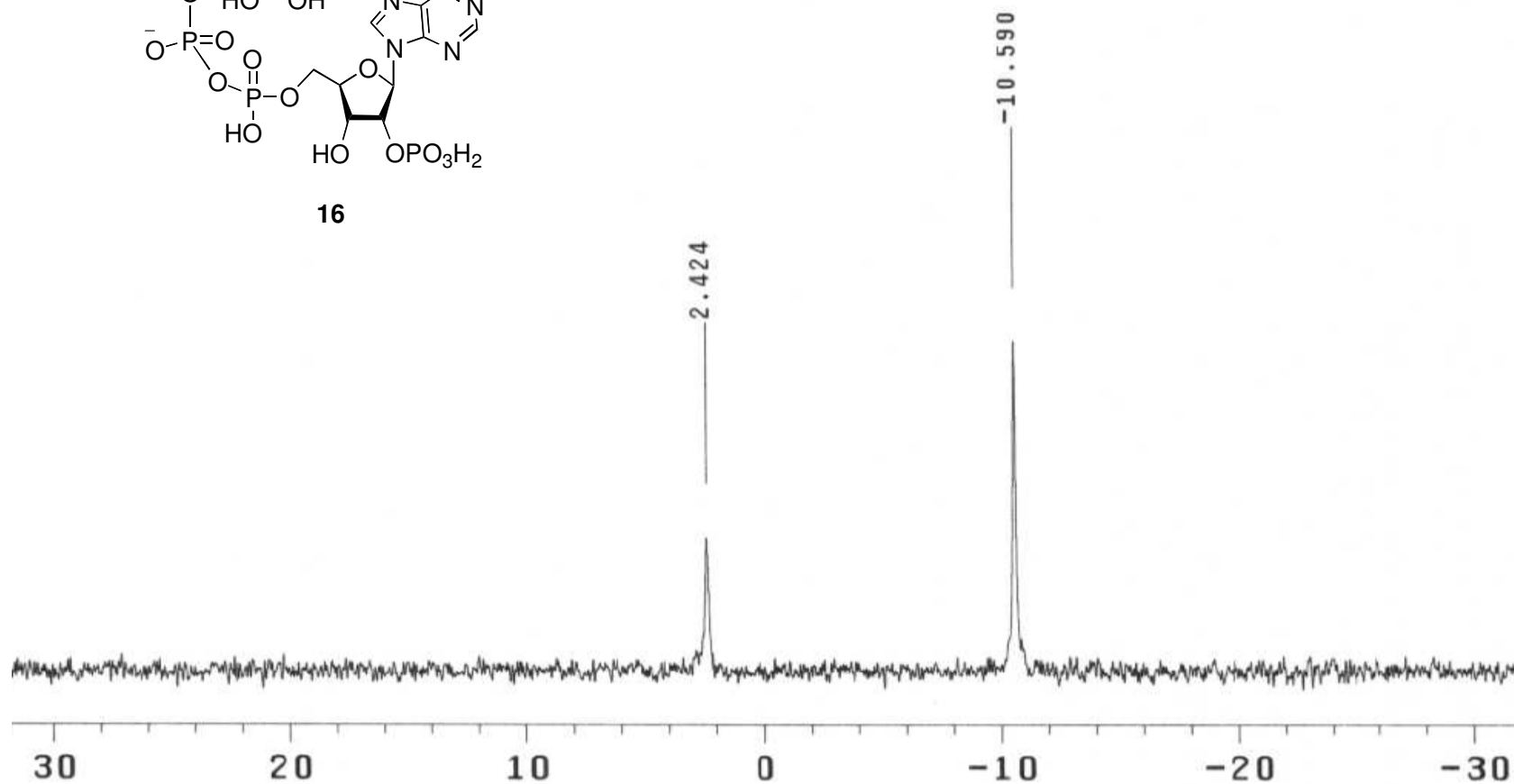
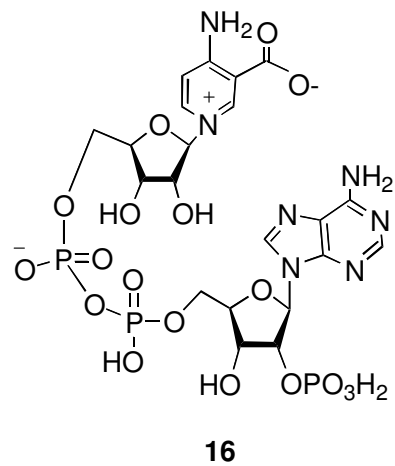


Figure S40. $^1\text{H-NMR}$ of **17**: 4-methyl-NAADP

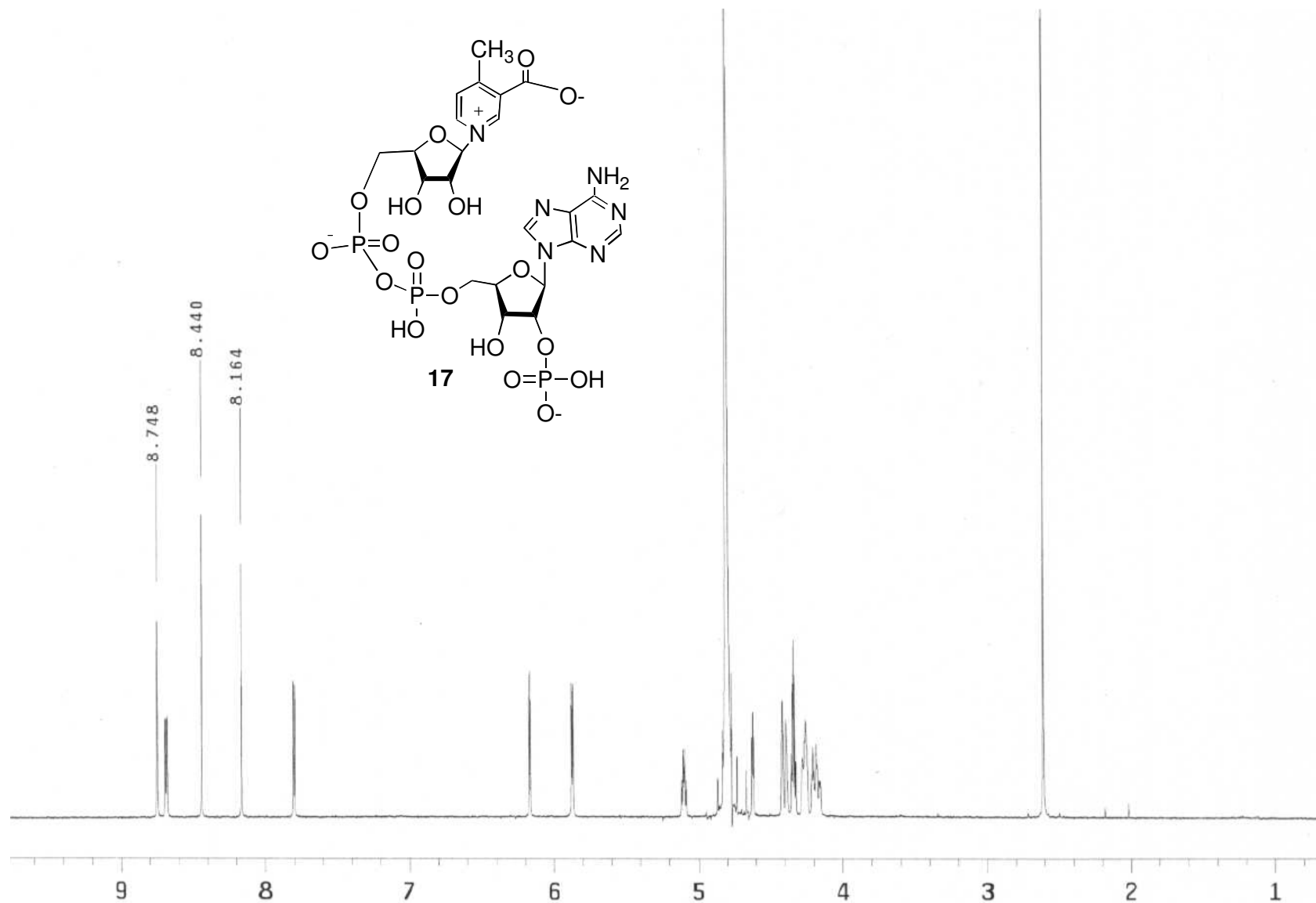


Figure S41. ^{31}P -NMR of **17**: 4-methyl-NAADP

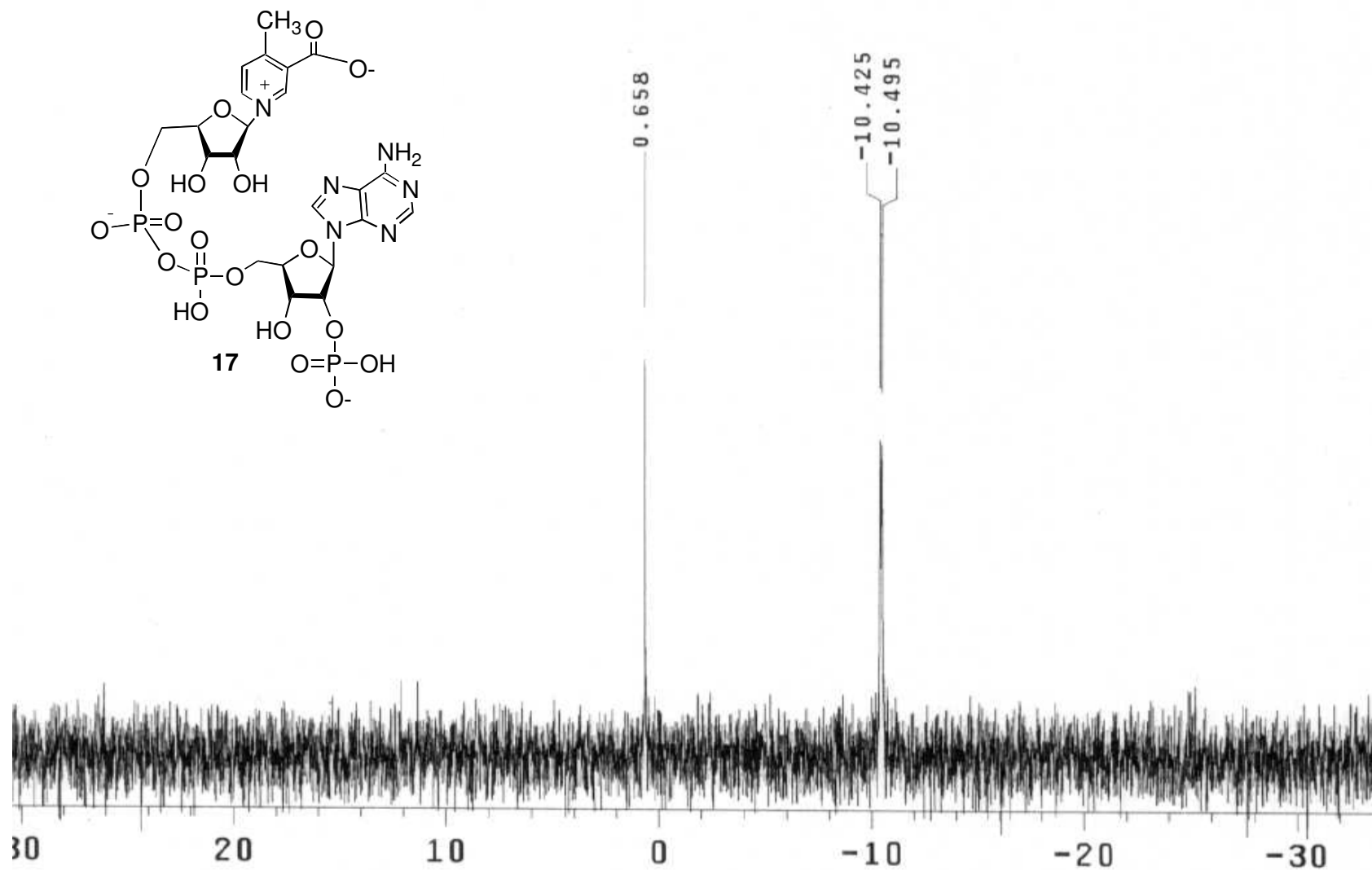


Figure S42. ¹H-NMR of **18**: 4-*n*-butyl-NAADP

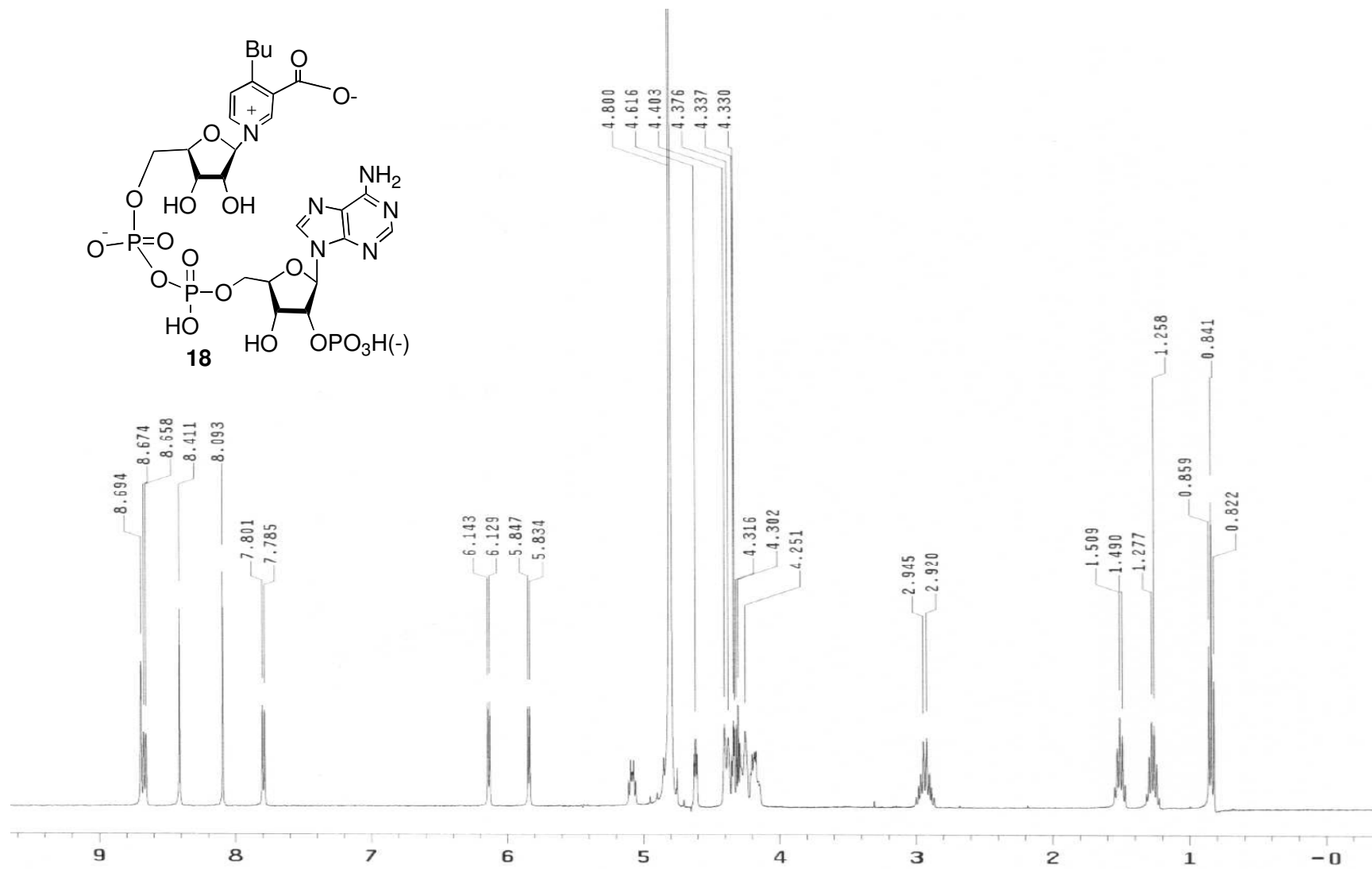


Figure S43. ¹H-NMR of **19**: 4-phenyl-NAADP

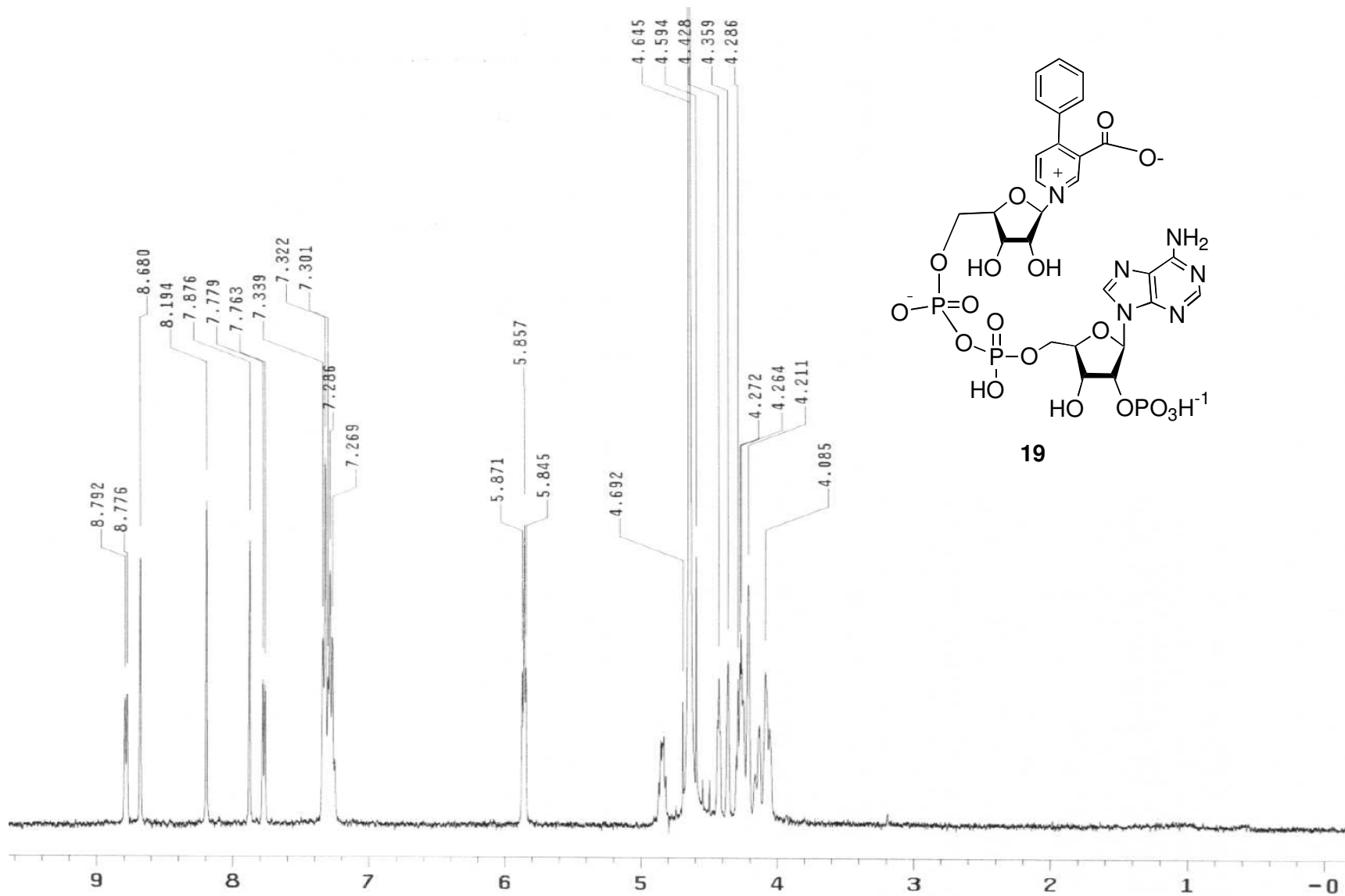


Figure S44. ^{31}P -NMR of **19**: 4-phenyl-NAADP

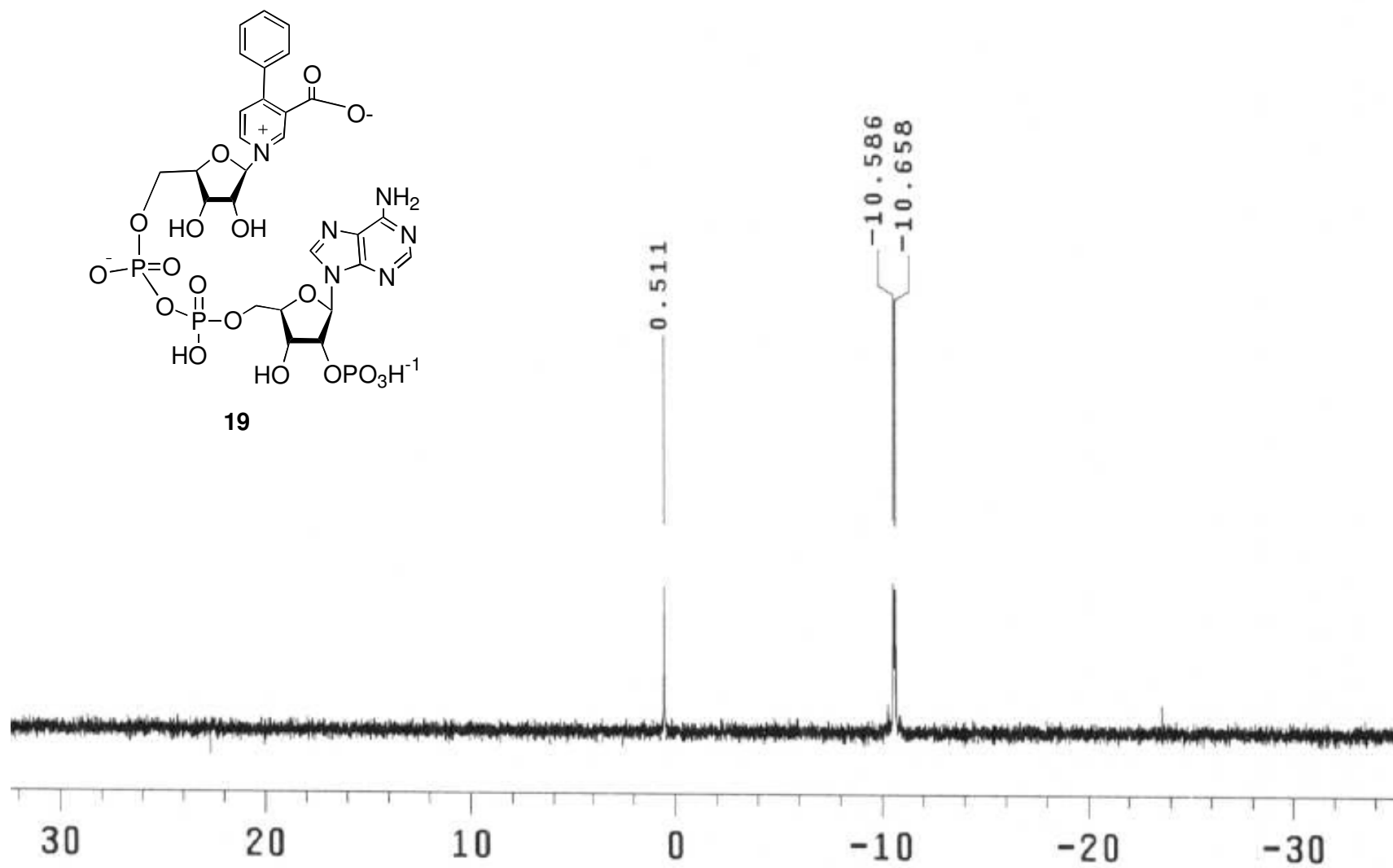


Figure S45. $^1\text{H-NMR}$ of **20**: 5-amino-NAADP

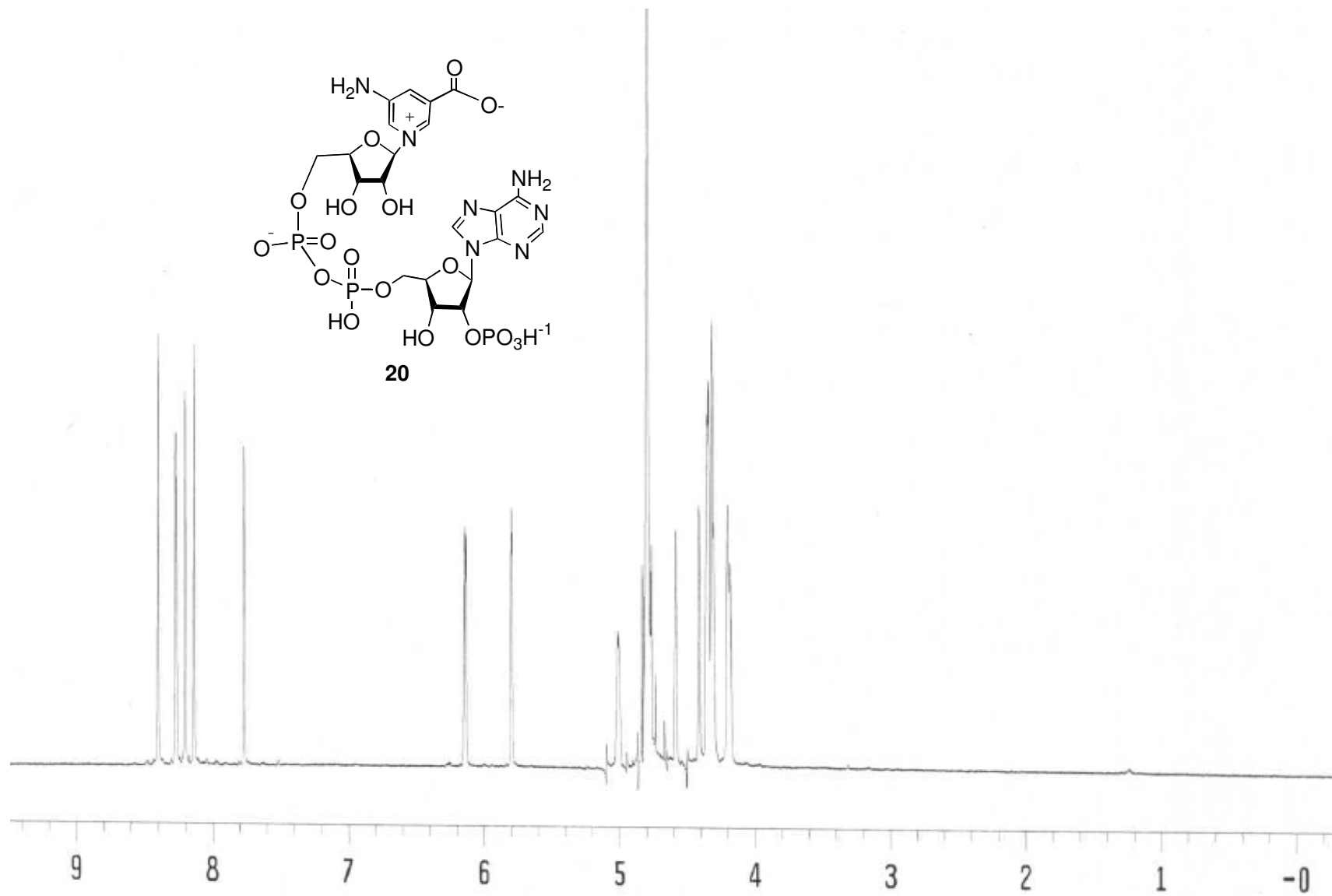


Figure S46. ^{31}P -NMR of **20**: 5-amino-NAADP

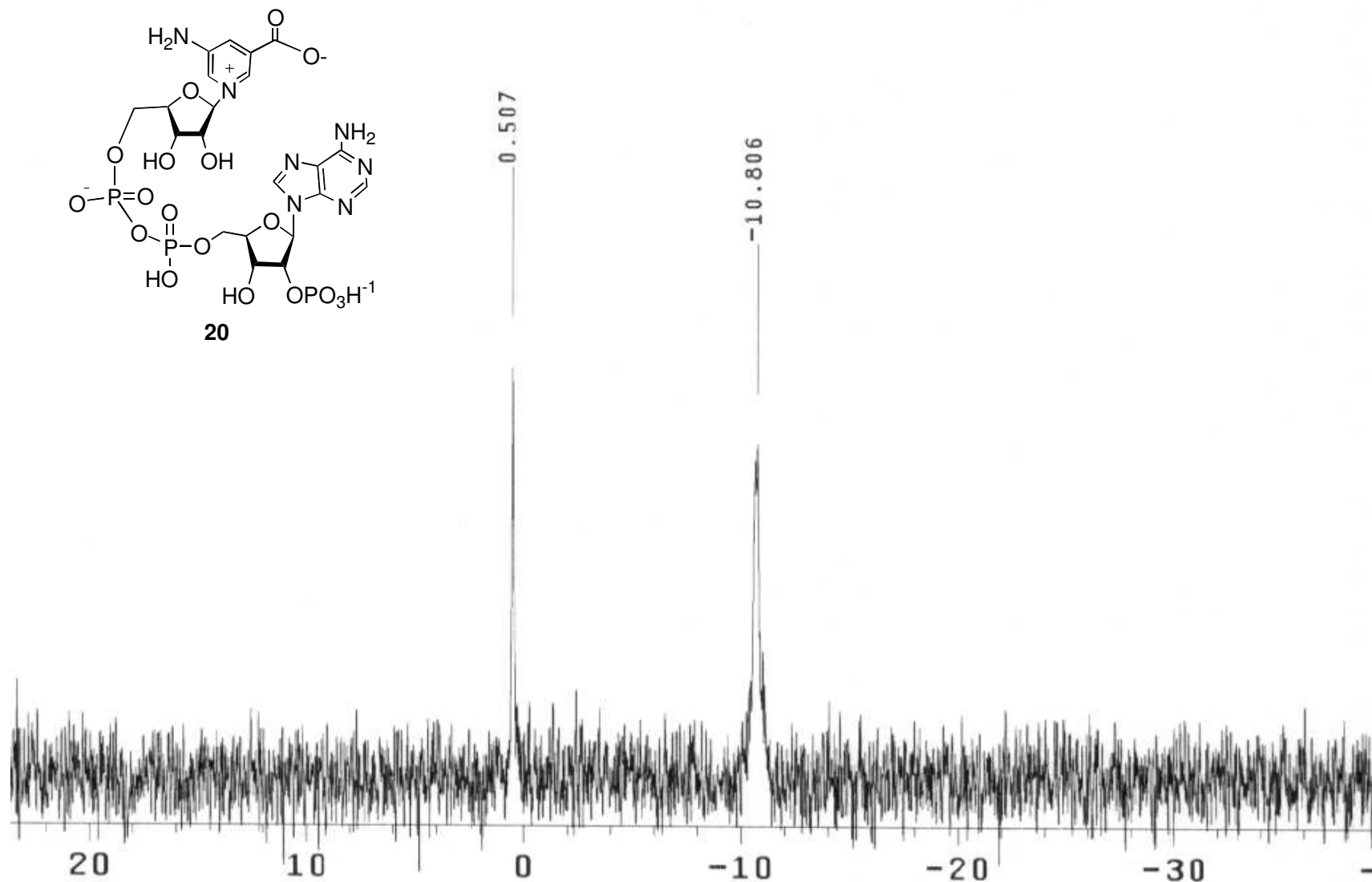


Figure S47. $^1\text{H-NMR}$ of **21**: 5-methyl-NAADP

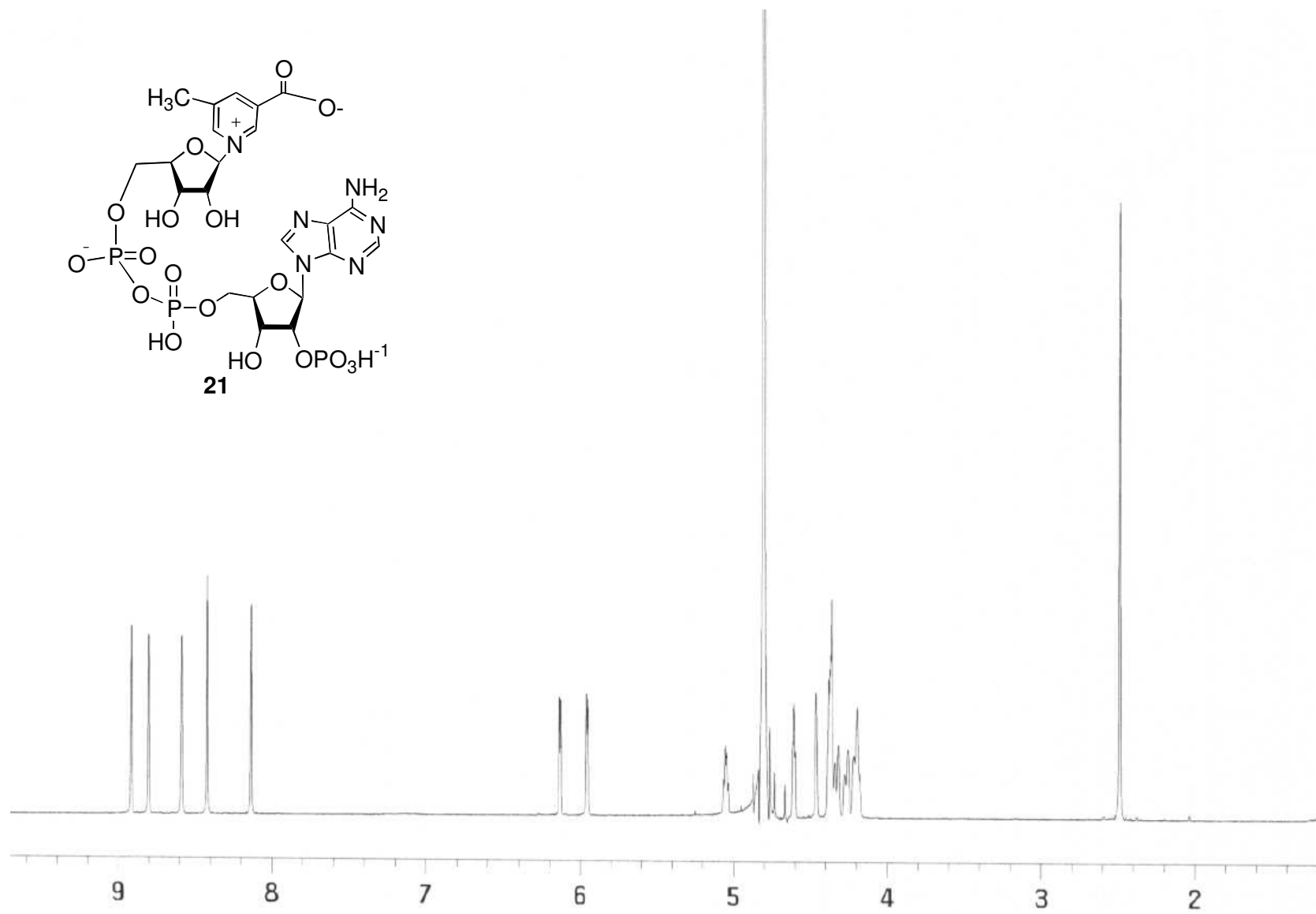


Figure S48. ^{31}P -NMR of **21**: 5-methyl-NAADP

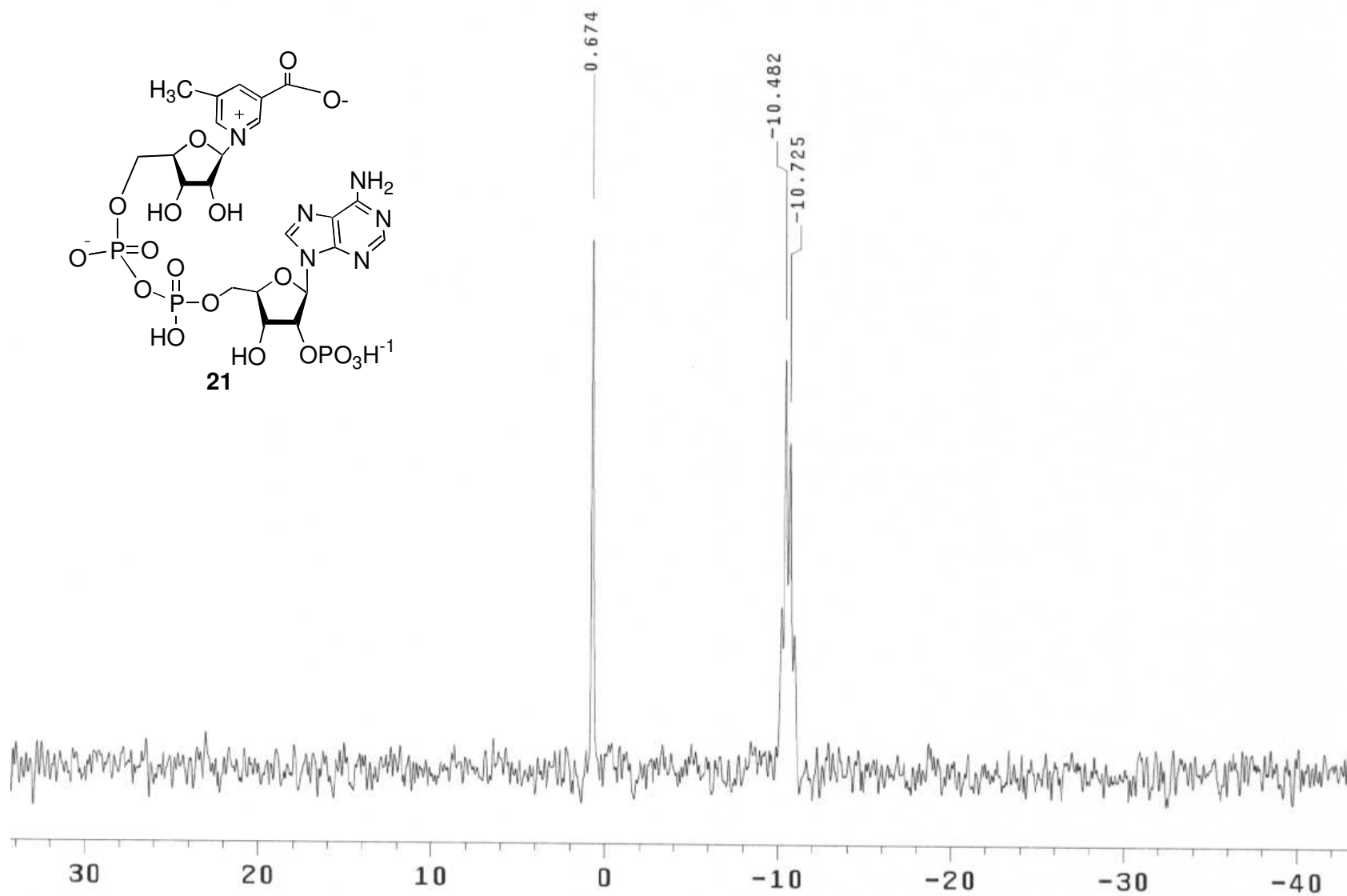


Figure S49. ¹H-NMR of **22**: 5-carboxy-NAADP

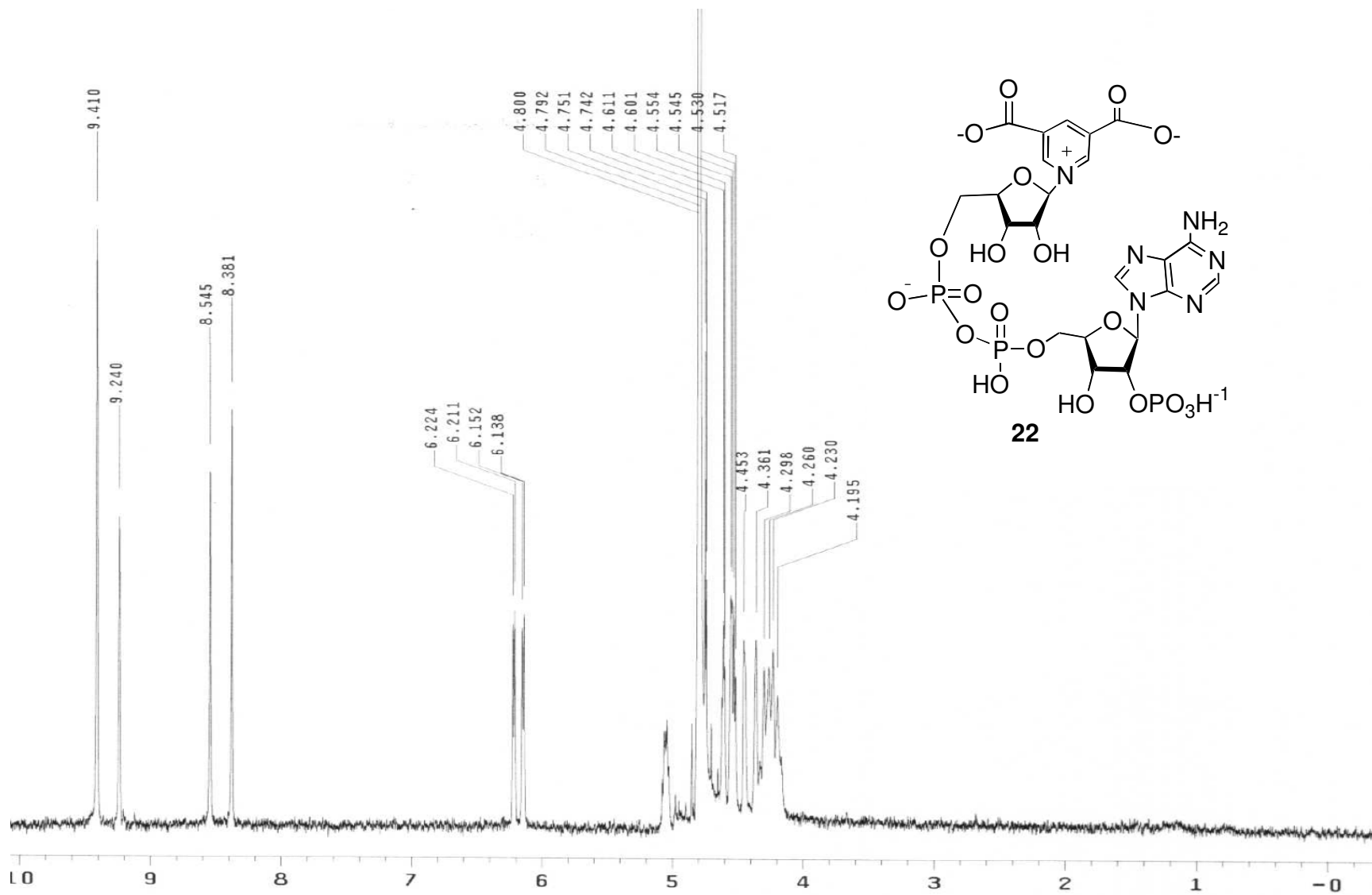


Figure S50. ^{31}P -NMR of **22**: 5-carboxy-NAADP

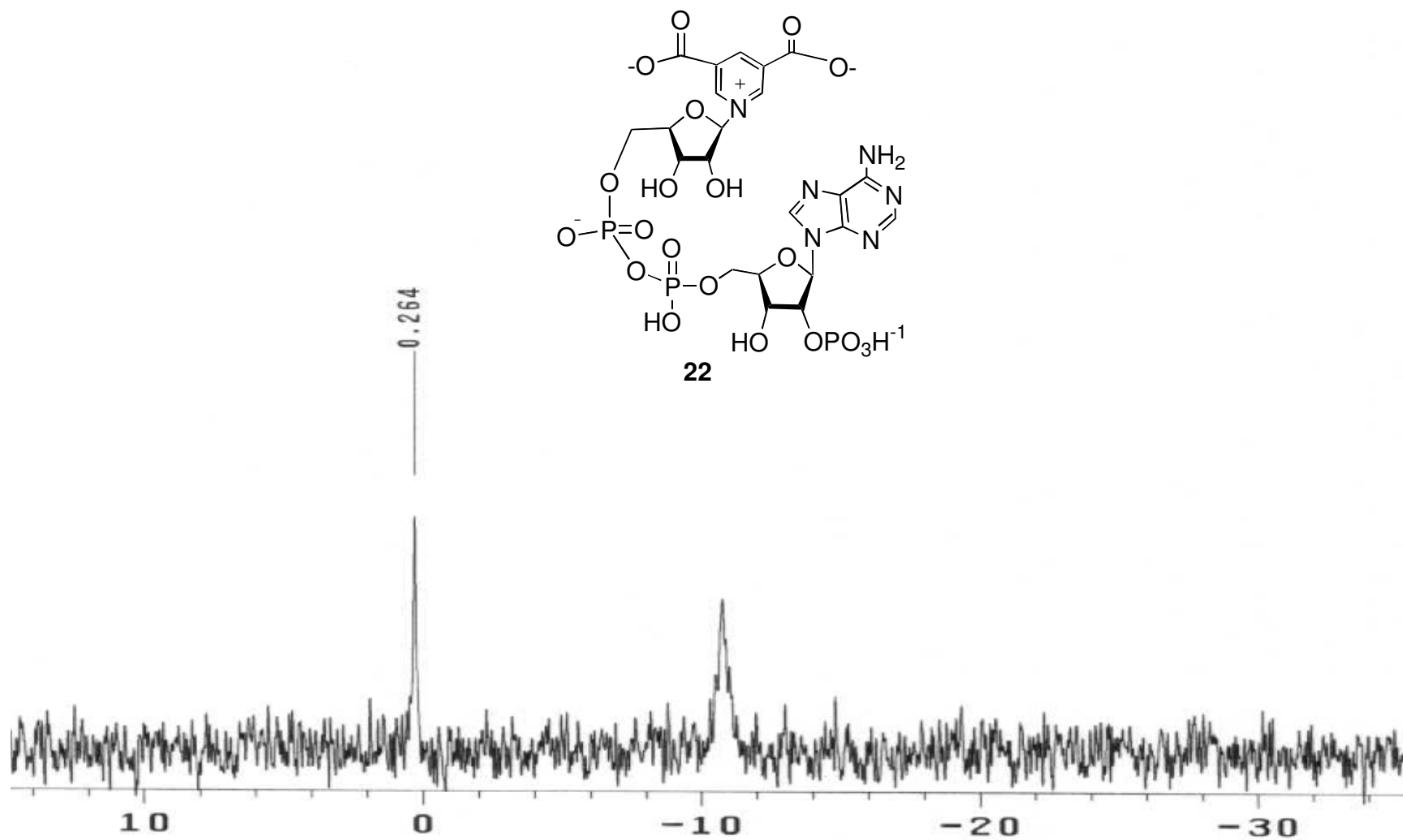


Figure S51. ¹H-NMR of **23**: 5-ethyl-NAADP

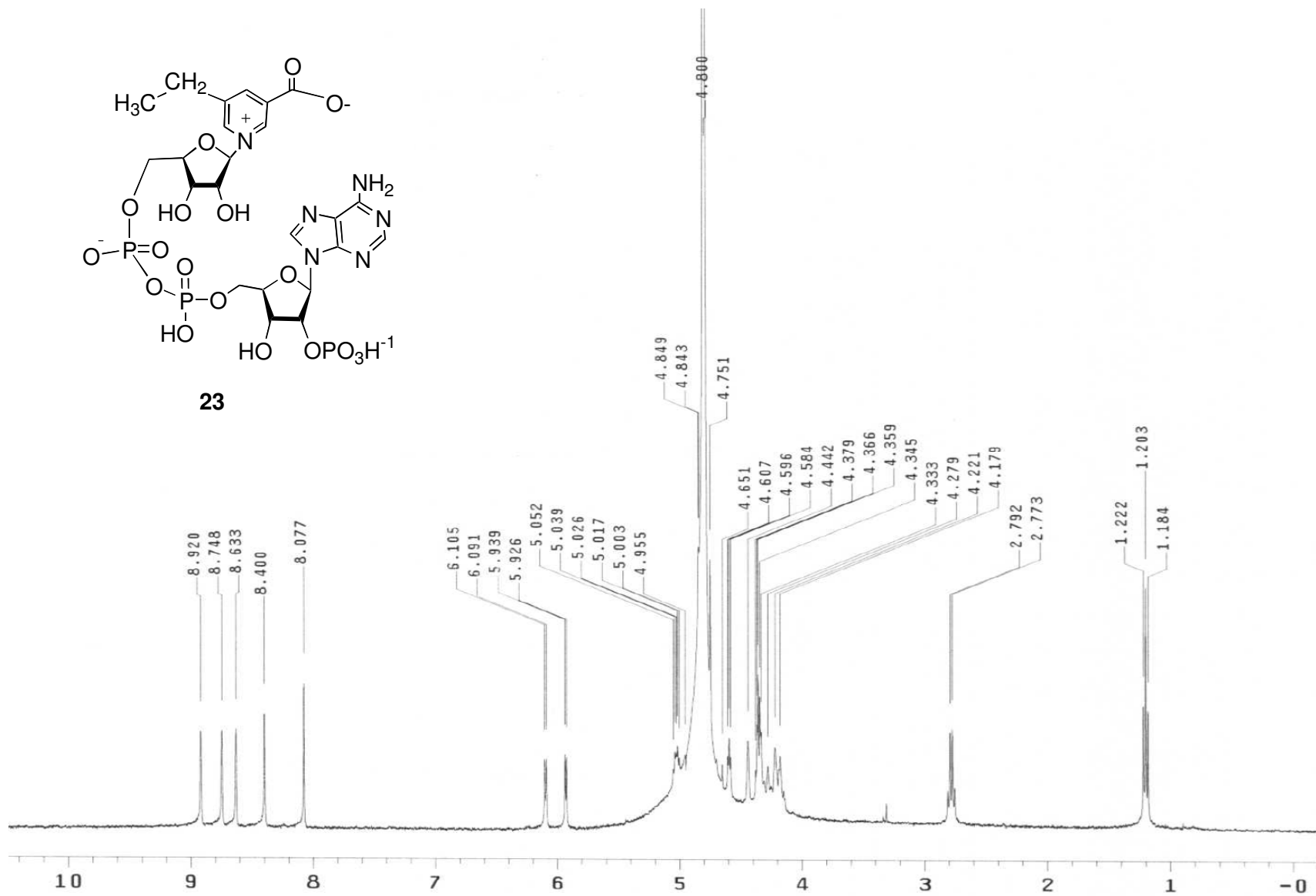


Figure S52. ^{31}P -NMR of **23**: 5-ethyl-NAADP

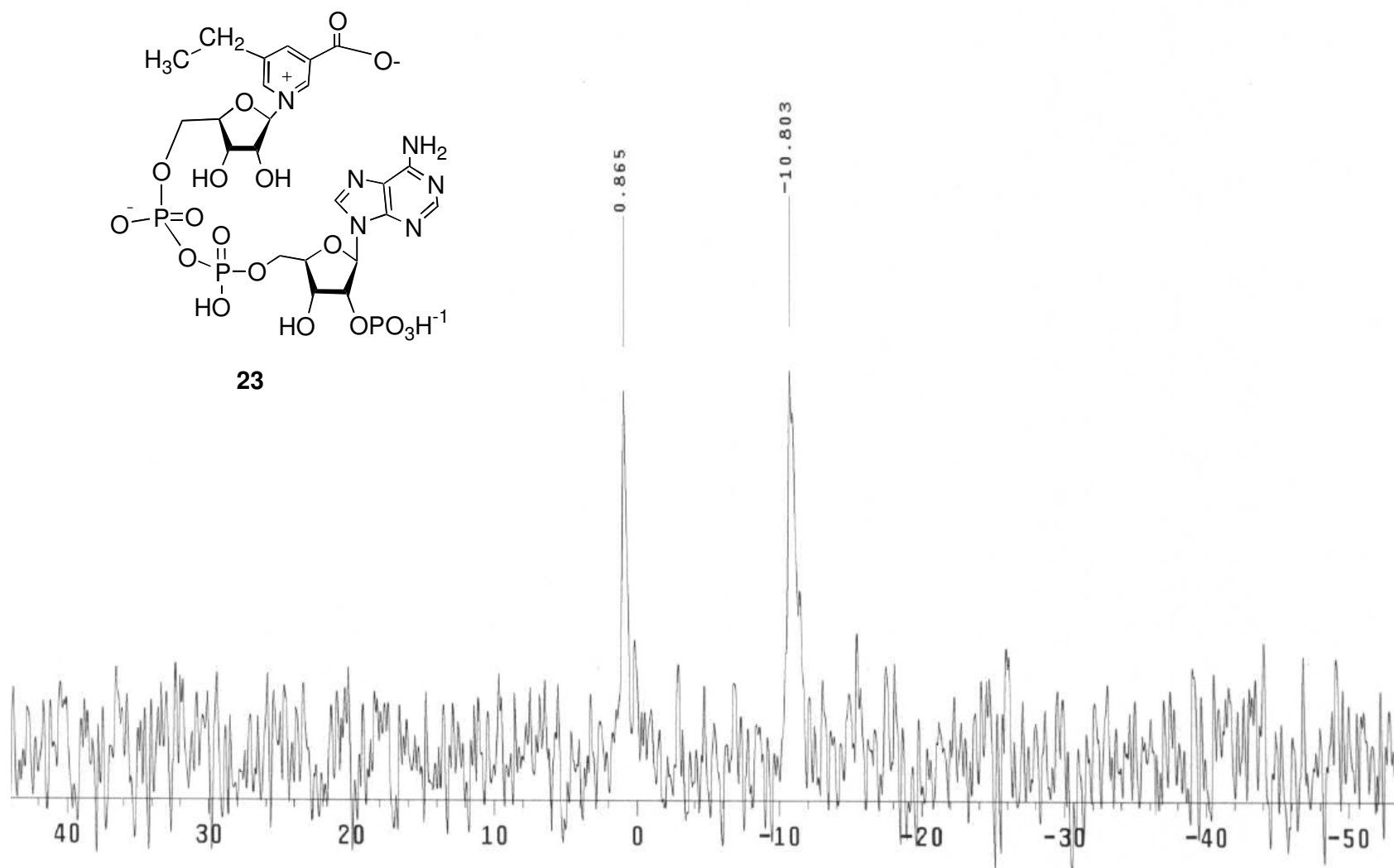


Figure S53. $^1\text{H-NMR}$ of **24**: 5-azido-NAADP

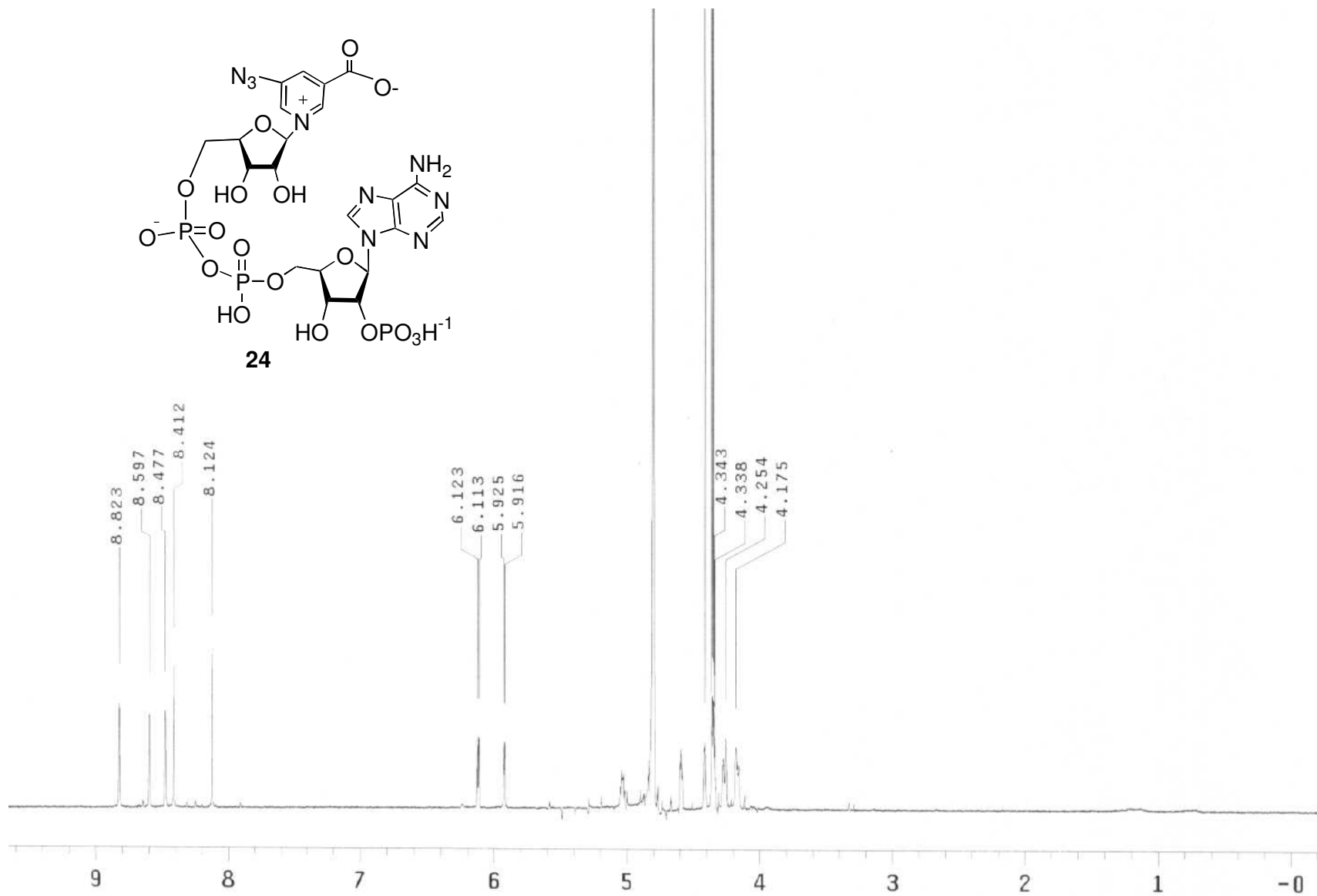
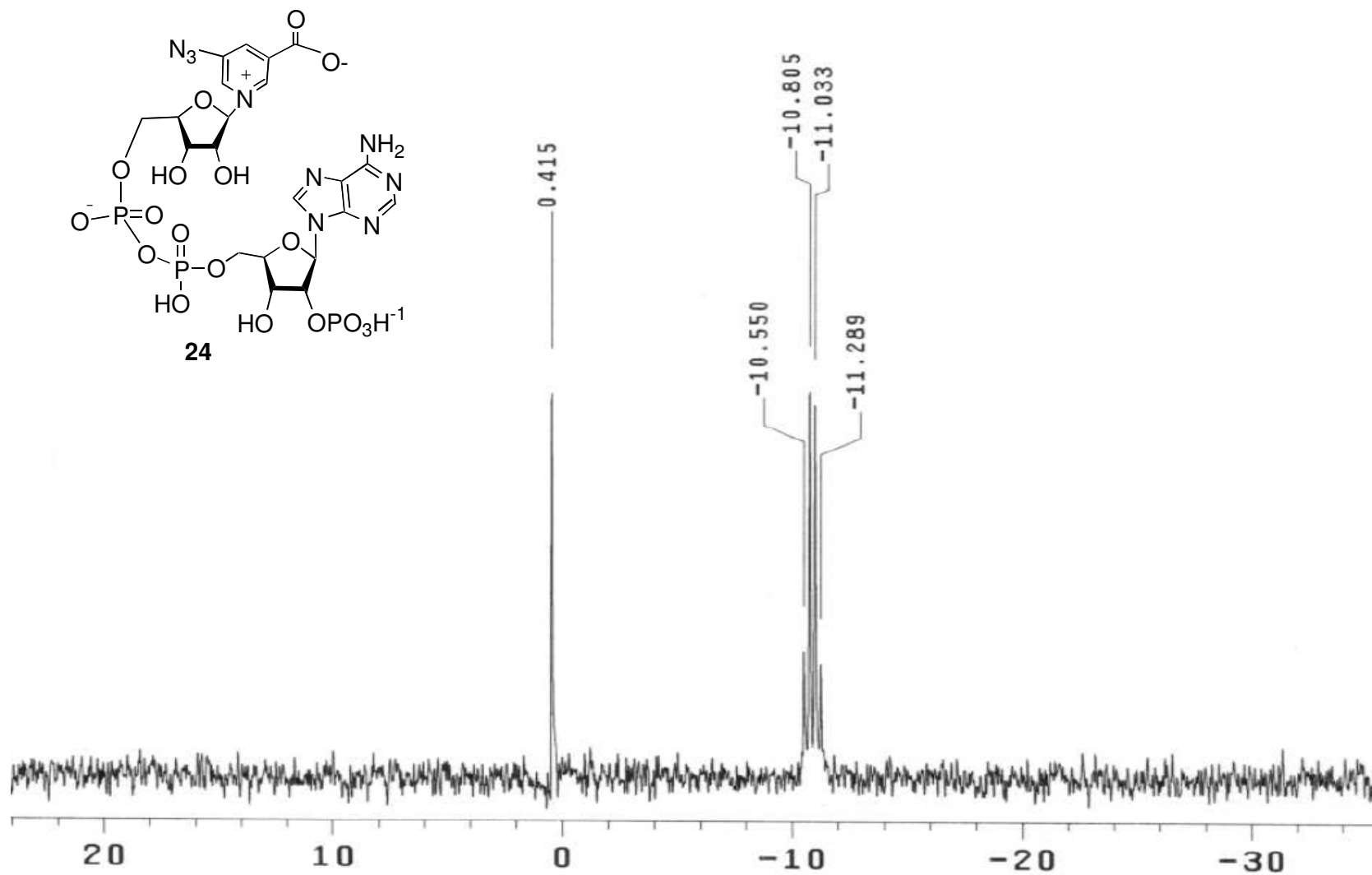


Figure S54. ^{31}P -NMR of **24**: 5-azido-NAADP



References

- (1) Axelson, J. T.; Bodley, J. W.; Walseth, T. F. A volatile liquid chromatography system for nucleotides. *Anal. Biochem.* **1981**, *116*, 357-360.