

Supporting Information

Evaluation of the interactions of hydrazide derivatives with acetic acid, and molecular modeling analysis of *N*-acetylated hydrazides

Hamid Beyzaei*, Sakineh Sheikh, Fereshteh Shiri*, Reza Aryan

Department of Chemistry, Faculty of Science, University of Zabol, Zabol, Iran

Email: hbeyzaei@uoz.ac.ir, hbeyzaei@yahoo.com; and fereshteh.shiri@gmail.com, fereshteh.shiri@uoz.ac.ir

Table of contents

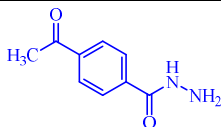
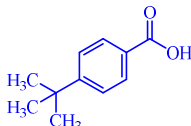
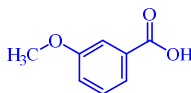
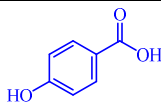
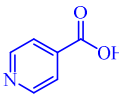
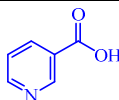
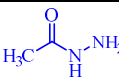
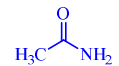
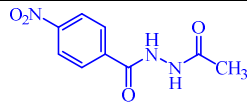
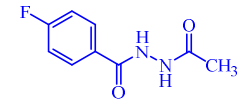
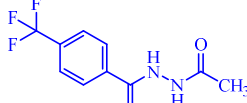
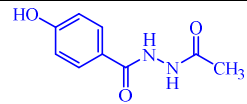
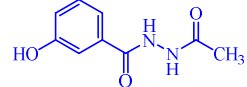
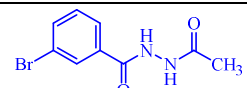
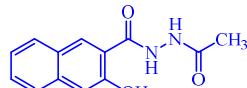
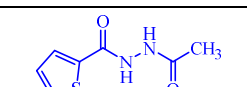
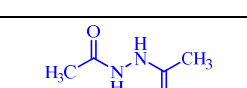
Entry	Description	Structure	Page
Fig. 1	¹ H NMR of 4-acetylbenzohydrazide (2a)		S4
Fig. 2	¹³ C NMR of 4-acetylbenzohydrazide (2a)		S5
Fig. 3	FT-IR of 4-acetylbenzohydrazide (2a)		S6
Fig. 4	¹ H NMR of 4-(<i>tert</i> -butyl)benzoic acid (2b)		S7
Fig. 5	¹³ C NMR of 4-(<i>tert</i> -butyl)benzoic acid (2b)		S8
Fig. 6	FT-IR of 4-(<i>tert</i> -butyl)benzoic acid (2b)		S9
Fig. 7	¹ H NMR of 3-methoxybenzoic acid (2c)		S10
Fig. 8	¹³ C NMR of 3-methoxybenzoic acid (2c)		S11
Fig. 9	FT-IR of 3-methoxybenzoic acid (2c)		S12
Fig. 10	¹ H NMR of 4-hydroxybenzoic acid (2d)		S13
Fig. 11	¹³ C NMR of 4-hydroxybenzoic acid (2d)		S14
Fig. 12	FT-IR of 4-hydroxybenzoic acid (2d)		S15
Fig. 13	¹ H NMR of isonicotinic acid (2e)		S16
Fig. 14	¹³ C NMR of isonicotinic acid (2e)		S17
Fig. 15	FT-IR of isonicotinic acid (2e)		S18
Fig. 16	¹ H NMR of nicotinic acid (2f)		S19
Fig. 17	¹³ C NMR of nicotinic acid (2f)		S20
Fig. 18	FT-IR of nicotinic acid (2f)		S21
Fig. 19	¹ H NMR of acetohydrazide (2g)		S22
Fig. 20	¹³ C NMR of acetohydrazide (2g)		S23
Fig. 21	FT-IR of acetohydrazide (2g)		S24
Fig. 22	¹ H NMR of acetamide (2h)		S25
Fig. 23	¹³ C NMR of acetamide (2h)		S26
Fig. 24	FT-IR of acetamide (2h)		S27

Fig. 25	¹ H NMR of <i>N'</i> -acetyl-4-nitrobenzohydrazide (2i)		S28
Fig. 26	¹³ C NMR of <i>N'</i> -acetyl-4-nitrobenzohydrazide (2i)		S29
Fig. 27	FT-IR of <i>N'</i> -acetyl-4-nitrobenzohydrazide (2i)		S30
Fig. 28	¹ H NMR of <i>N'</i> -acetyl-4-fluorobenzohydrazide (2j)		S31
Fig. 29	¹³ C NMR of <i>N'</i> -acetyl-4-fluorobenzohydrazide (2j)		S32
Fig. 30	FT-IR of <i>N'</i> -acetyl-4-fluorobenzohydrazide (2j)		S33
Fig. 31	¹ H NMR of <i>N'</i> -acetyl-4-(trifluoromethyl)benzohydrazide (2k)		S34
Fig. 32	¹³ C NMR of <i>N'</i> -acetyl-4-(trifluoromethyl)benzohydrazide (2k)		S35
Fig. 33	FT-IR of <i>N'</i> -acetyl-4-(trifluoromethyl)benzohydrazide (2k)		S36
Fig. 34	¹ H NMR of <i>N'</i> -acetyl-4-hydroxybenzohydrazide (2l)		S37
Fig. 35	¹³ C NMR of <i>N'</i> -acetyl-4-hydroxybenzohydrazide (2l)		S38
Fig. 36	FT-IR of <i>N'</i> -acetyl-4-hydroxybenzohydrazide (2l)		S39
Fig. 37	¹ H NMR of <i>N'</i> -acetyl-3-hydroxybenzohydrazide (2m)		S40
Fig. 38	¹³ C NMR of <i>N'</i> -acetyl-3-hydroxybenzohydrazide (2m)		S41
Fig. 39	FT-IR of <i>N'</i> -acetyl-3-hydroxybenzohydrazide (2m)		S42
Fig. 40	¹ H NMR of <i>N'</i> -acetyl-3-bromobenzohydrazide (2n)		S43
Fig. 41	¹³ C NMR of <i>N'</i> -acetyl-3-bromobenzohydrazide (2n)		S44
Fig. 42	FT-IR of <i>N'</i> -acetyl-3-bromobenzohydrazide (2n)		S45
Fig. 43	¹ H NMR of <i>N'</i> -acetyl-3-hydroxy-2-naphthohydrazide (2o)		S46
Fig. 44	¹³ C NMR of <i>N'</i> -acetyl-3-hydroxy-2-naphthohydrazide (2o)		S47
Fig. 45	FT-IR of <i>N'</i> -acetyl-3-hydroxy-2-naphthohydrazide (2o)		S48
Fig. 46	¹ H NMR of <i>N'</i> -acetylthiophene-2-carbohydrazide (2p)		S49
Fig. 47	¹³ C NMR of <i>N'</i> -acetylthiophene-2-carbohydrazide (2p)		S50
Fig. 48	FT-IR of <i>N'</i> -acetylthiophene-2-carbohydrazide (2p)		S51
Fig. 49	¹ H NMR of <i>N'</i> -acetylacetohydrazide (2q)		S52
Fig. 50	¹³ C NMR of <i>N'</i> -acetylacetohydrazide (2q)		S53
Fig. 51	FT-IR of <i>N'</i> -acetylacetohydrazide (2q)		S54

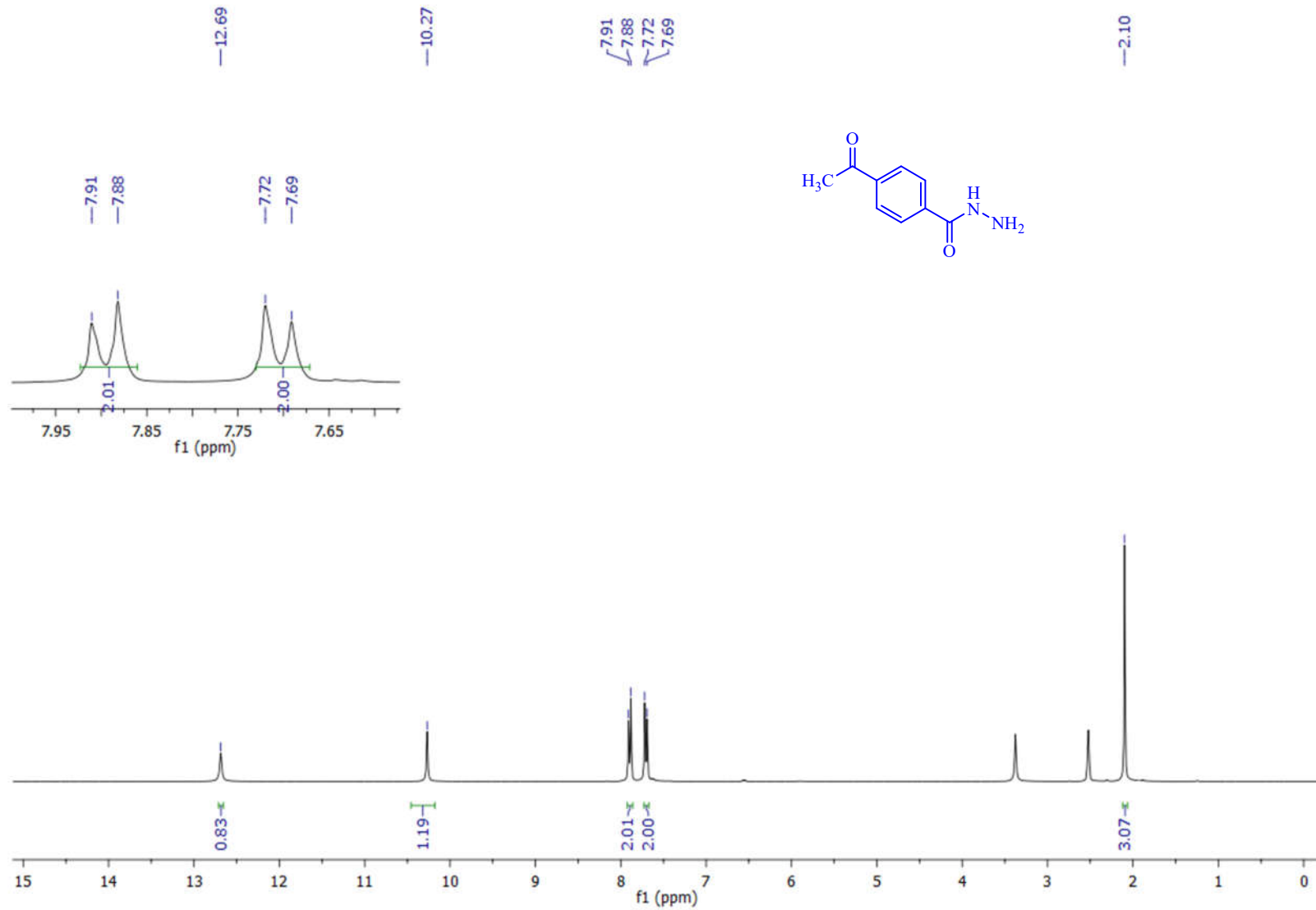


Fig. 1 ^1H NMR of 4-acetylbenzohydrazide (**2a**)

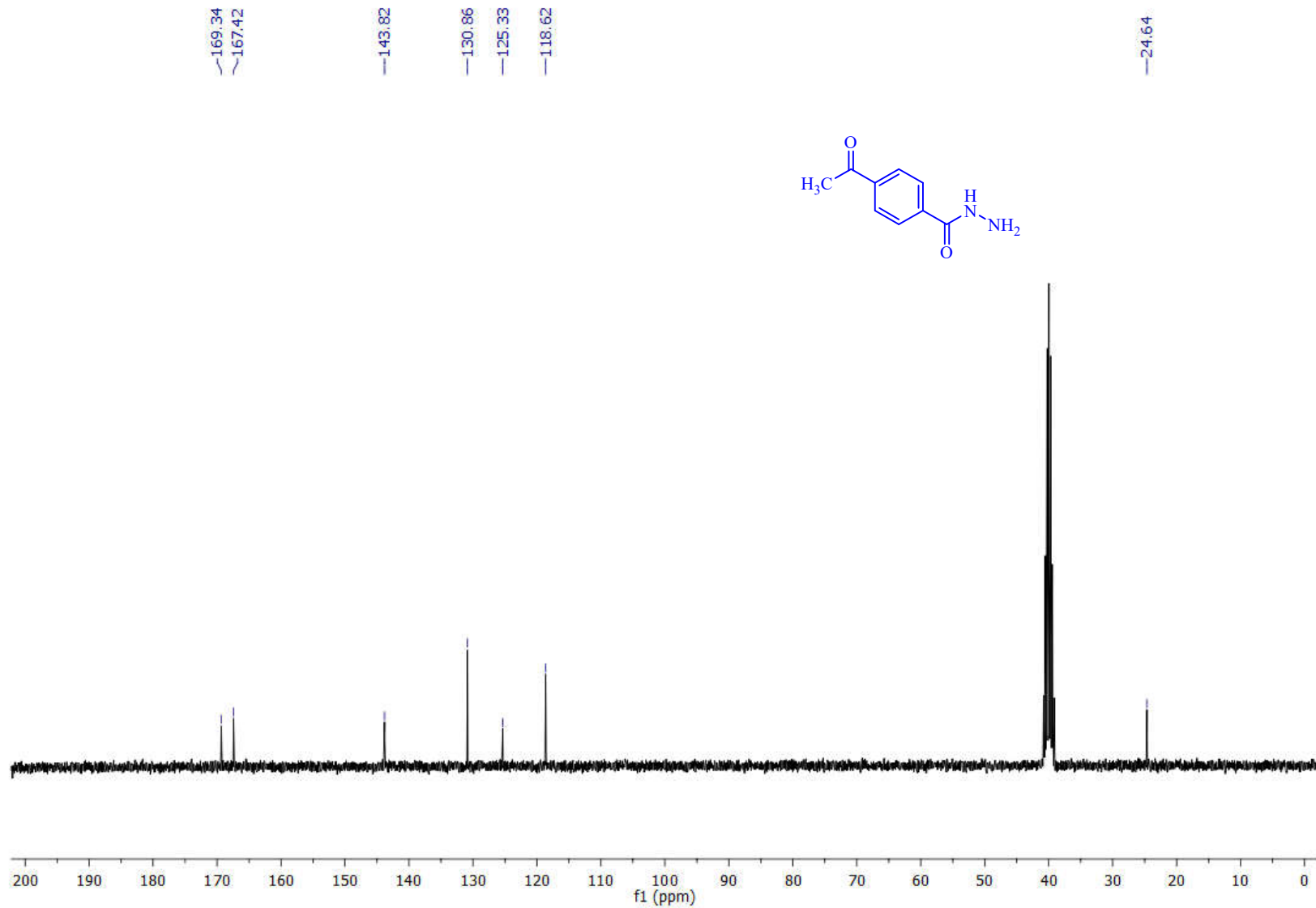


Fig. 2 ^{13}C NMR of 4-acetylbenzohydrazide (**2a**)

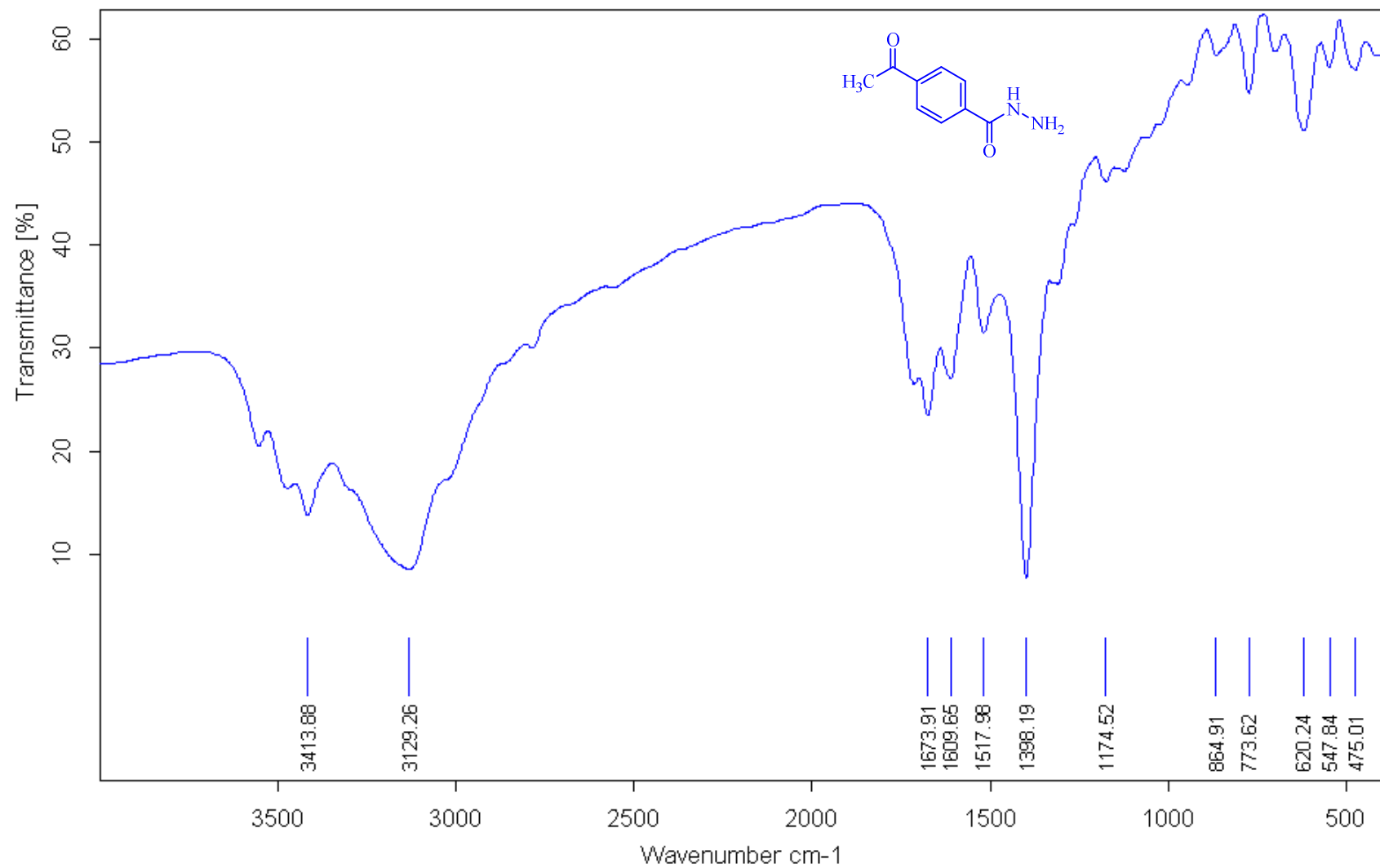


Fig. 3 FT-IR of 4-acetylbenzohydrazide (**2a**)

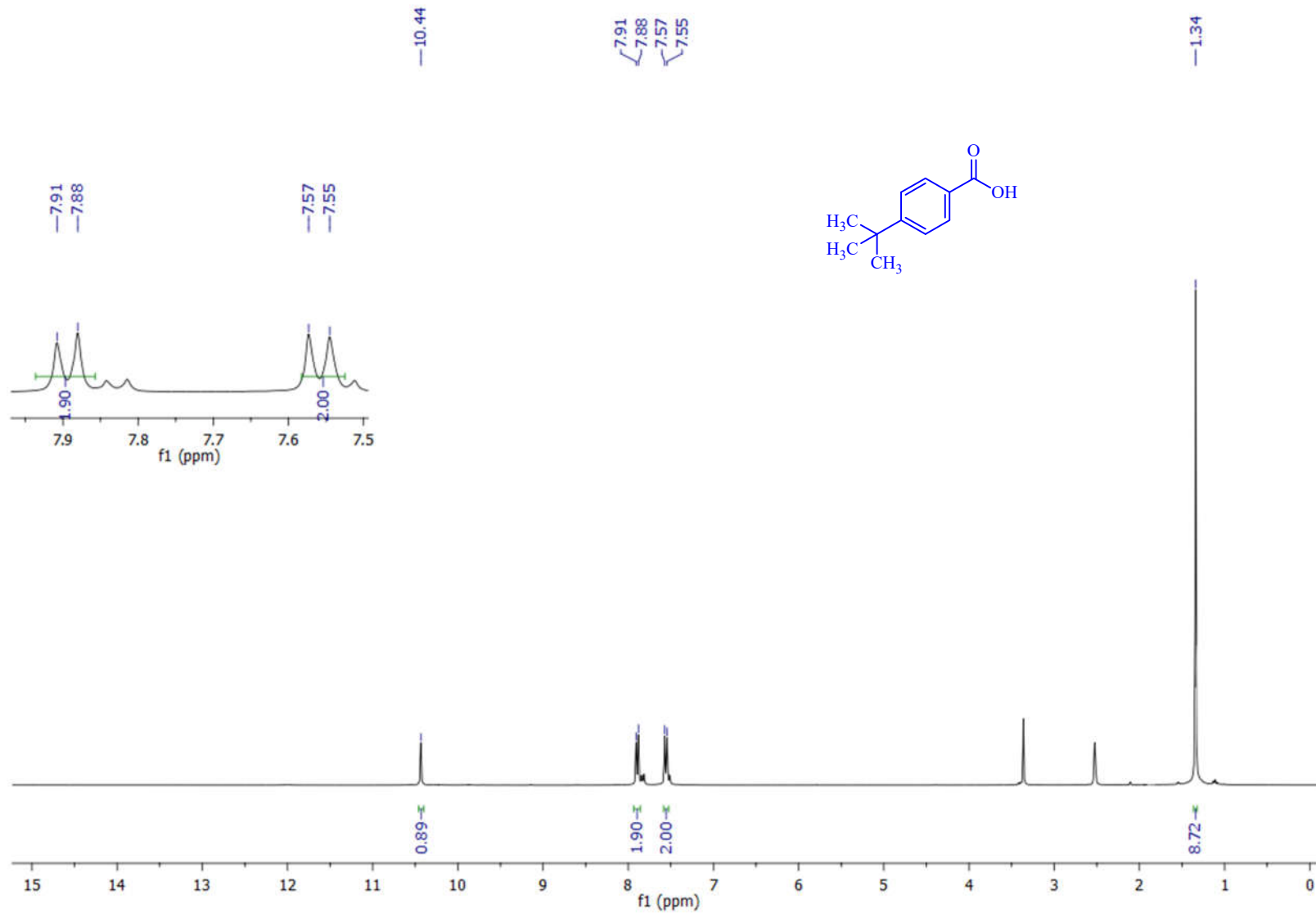


Fig. 4 ^1H NMR of 4-(*tert*-butyl)benzoic acid (**2b**)

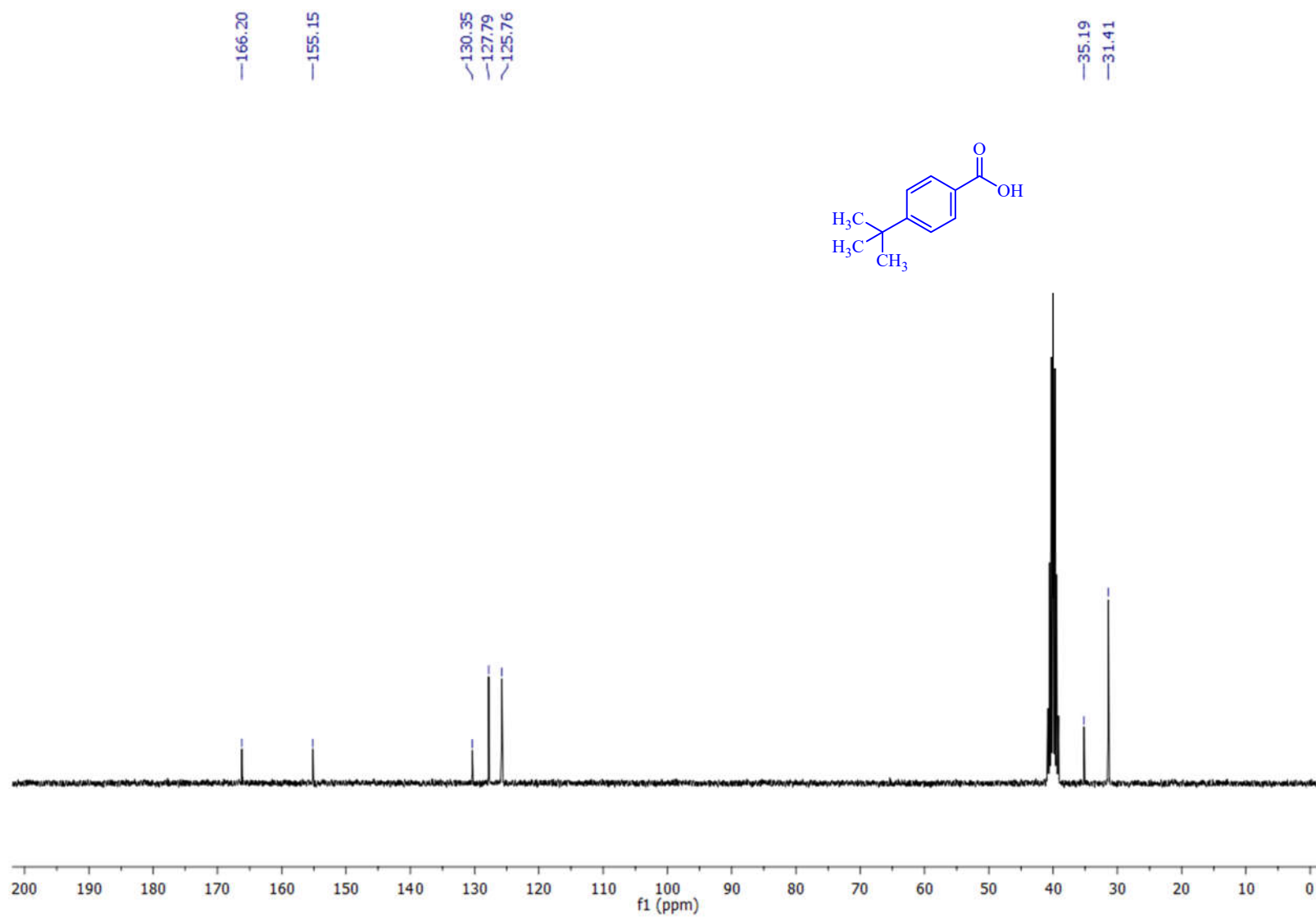


Fig. 5 ^{13}C NMR of 4-(*tert*-butyl)benzoic acid (**2b**)

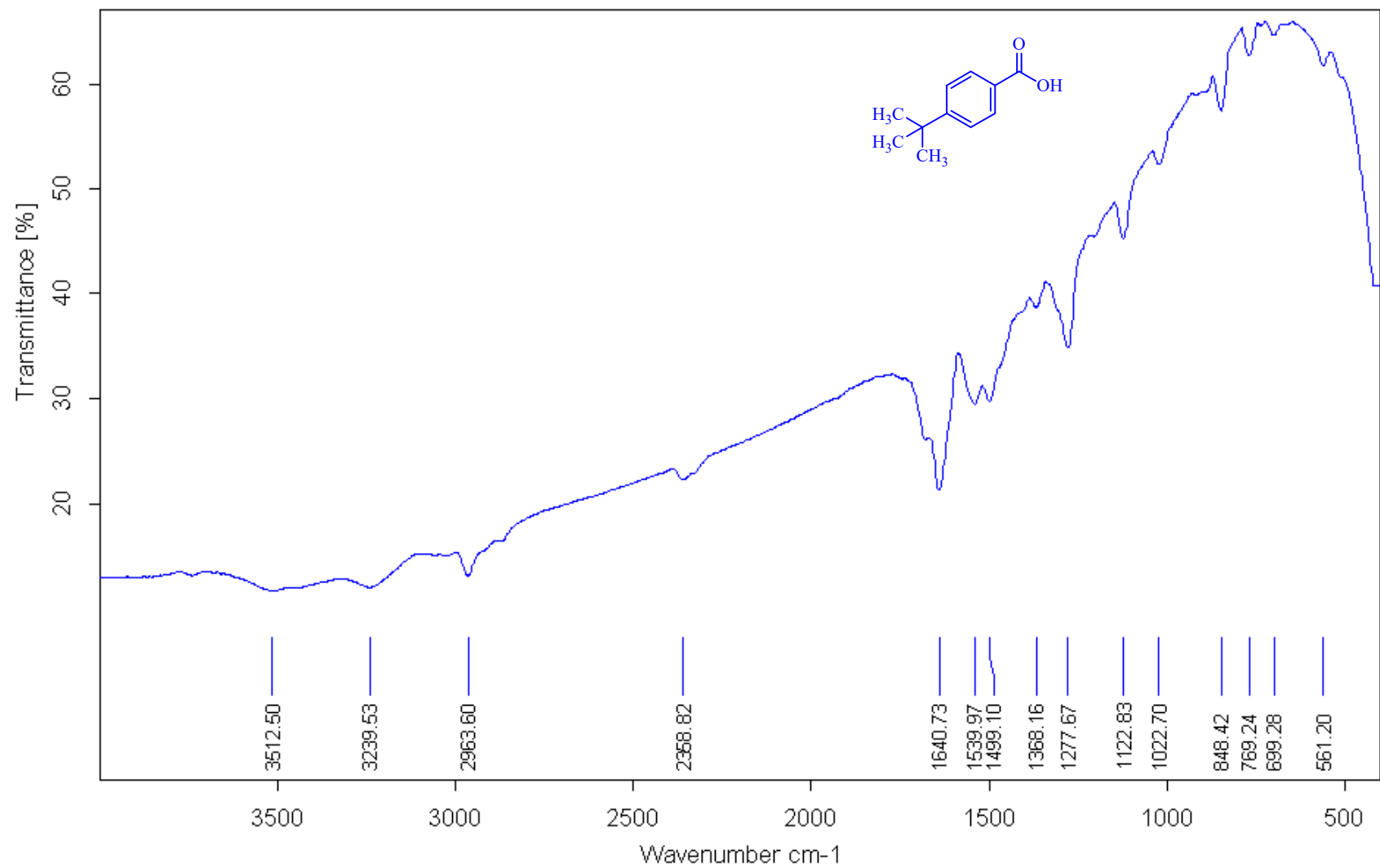


Fig. 6 FT-IR of 4-(*tert*-butyl)benzoic acid (**2b**)

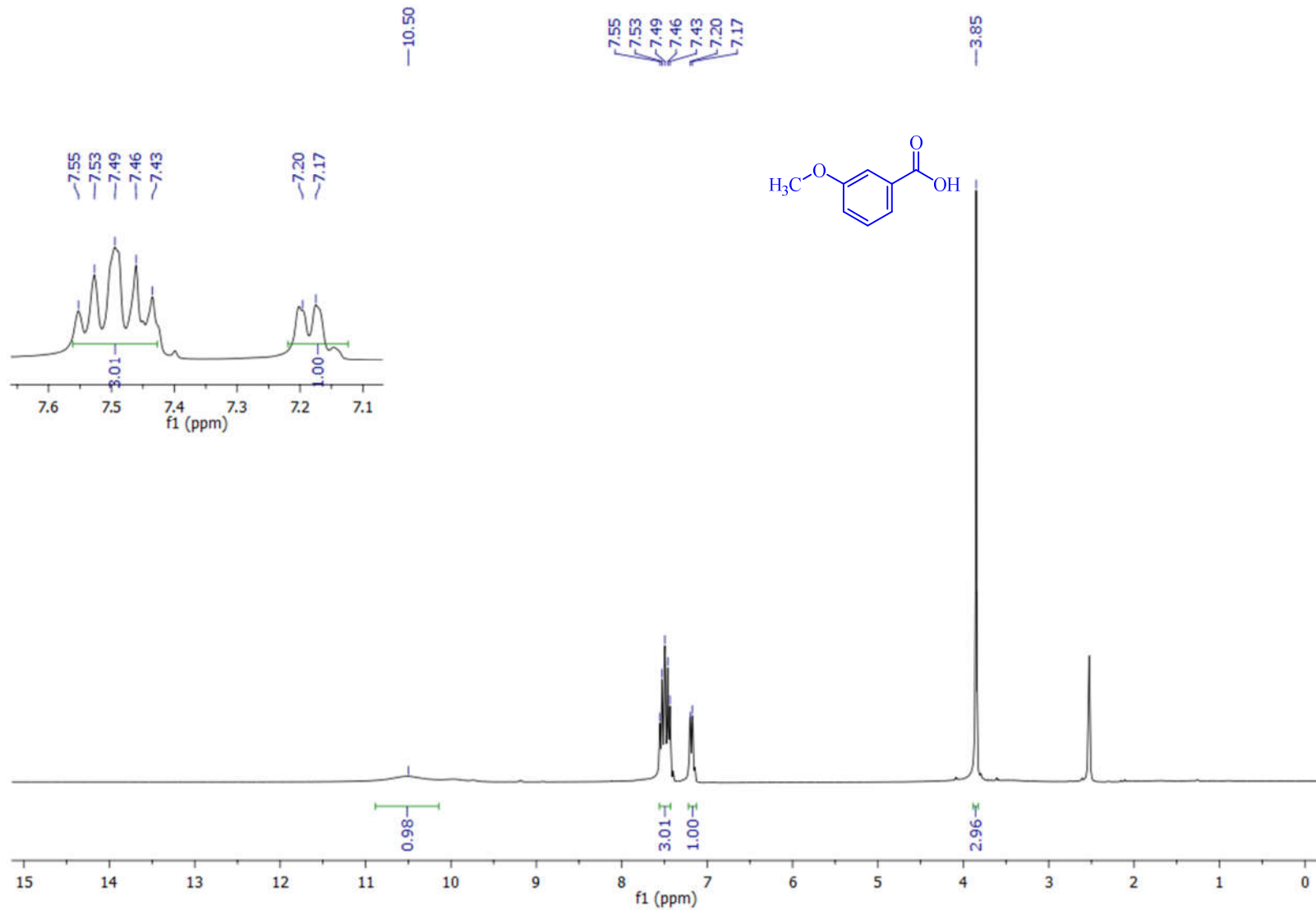


Fig. 7 ^1H NMR of 3-methoxybenzoic acid (**2c**)

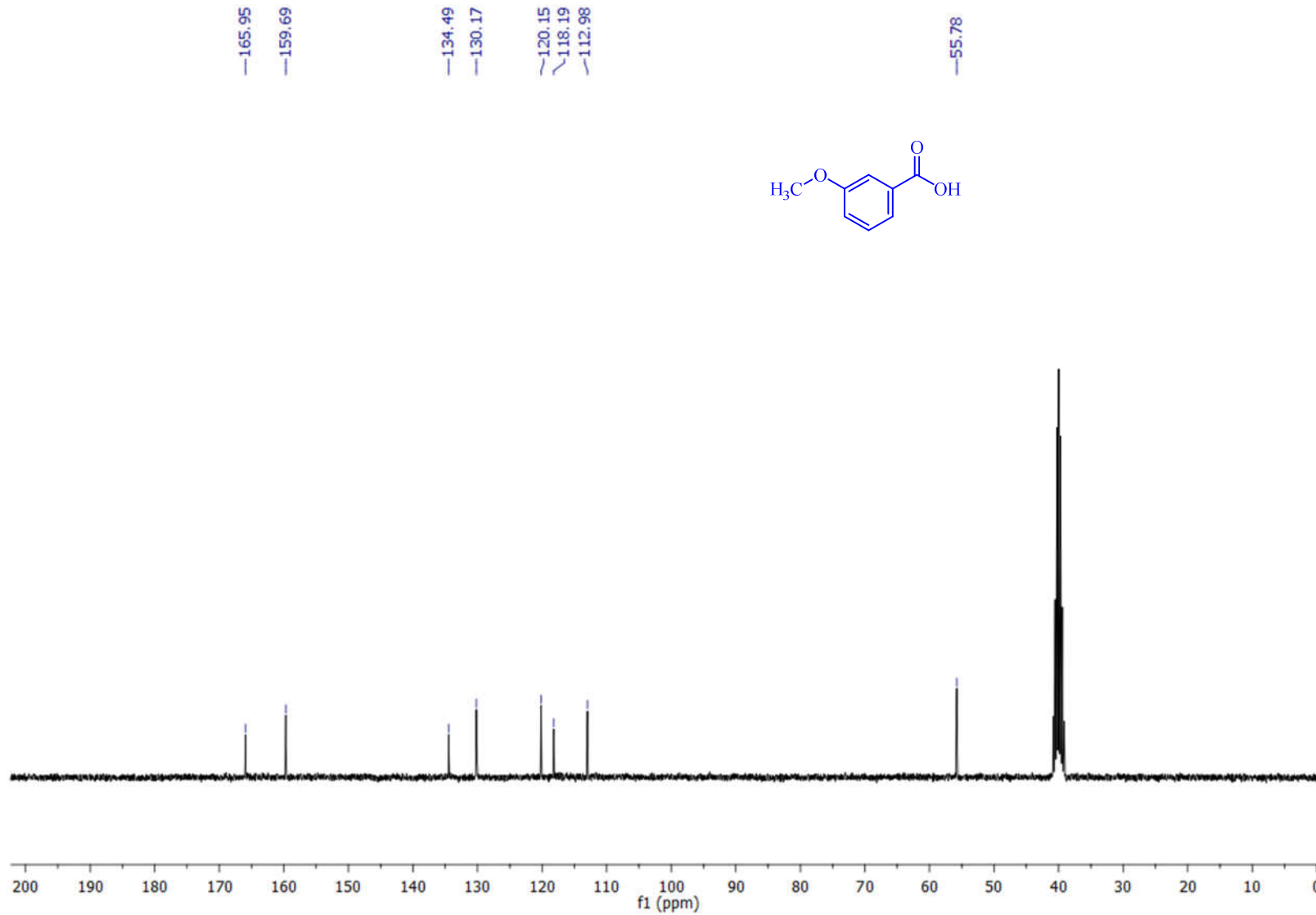


Fig. 8 ^{13}C NMR of 3-methoxybenzoic acid (**2c**)

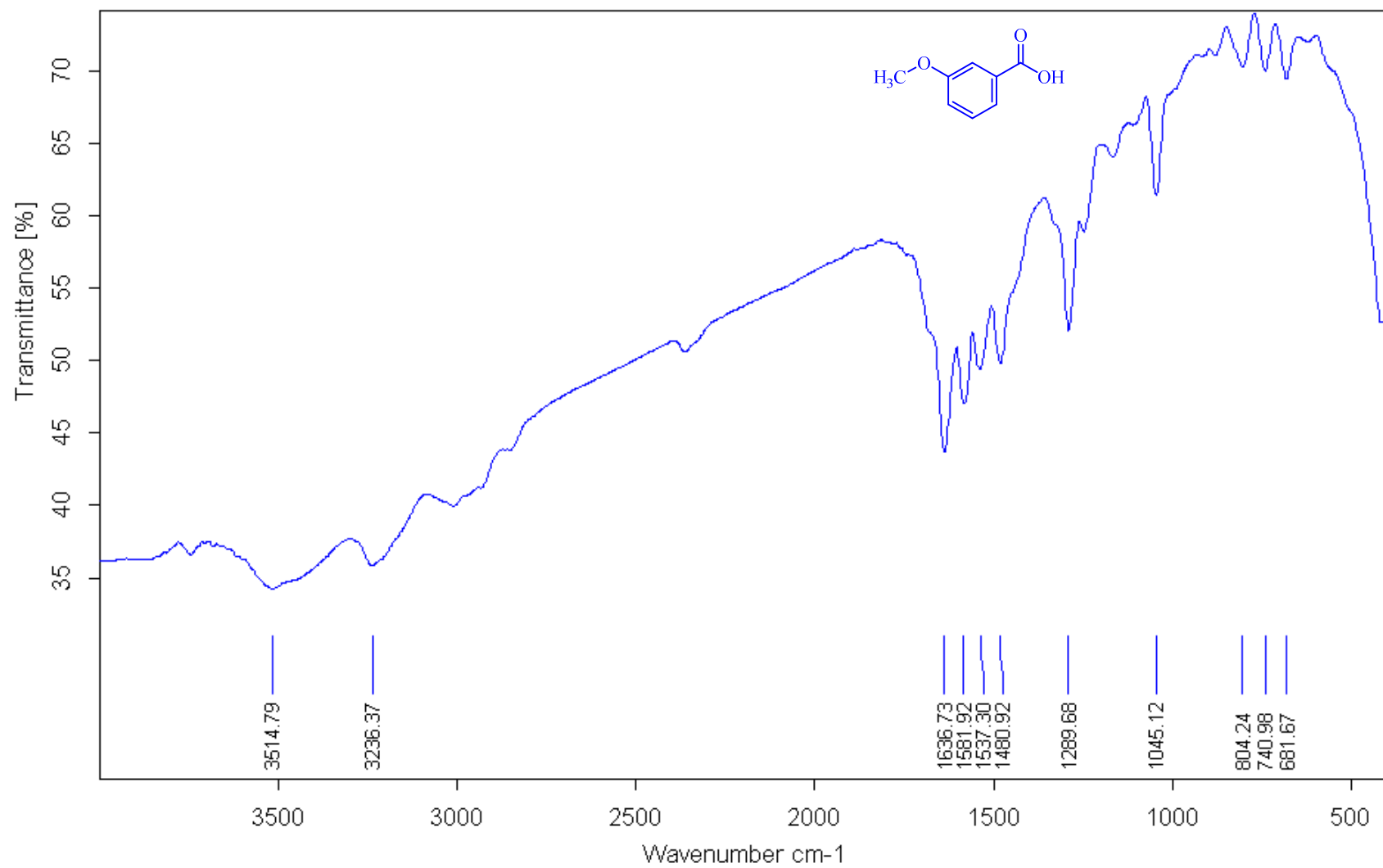


Fig. 9 FT-IR of 3-methoxybenzoic acid (**2c**)

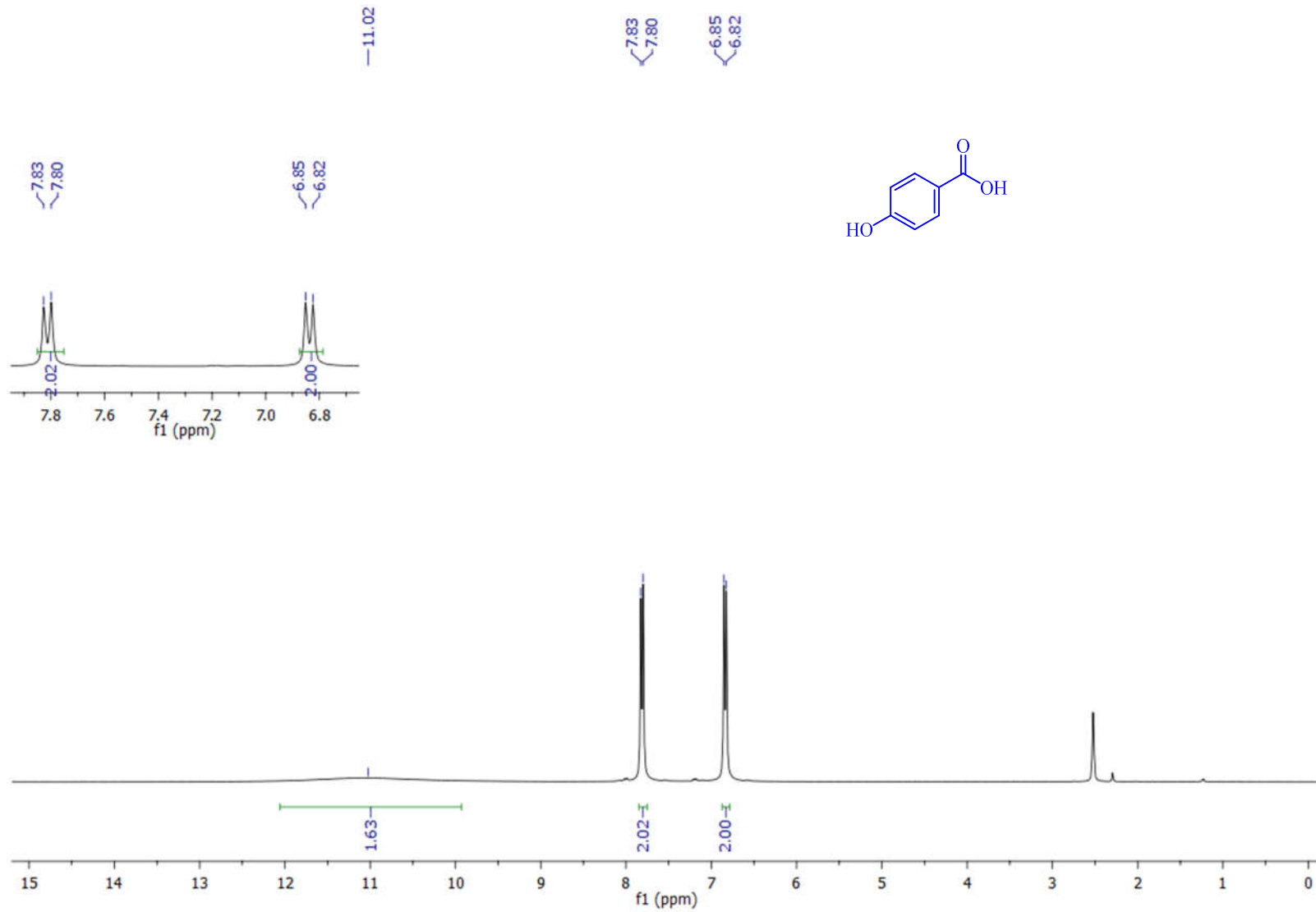


Fig. 10 ^1H NMR of 4-hydroxybenzoic acid (**2d**)

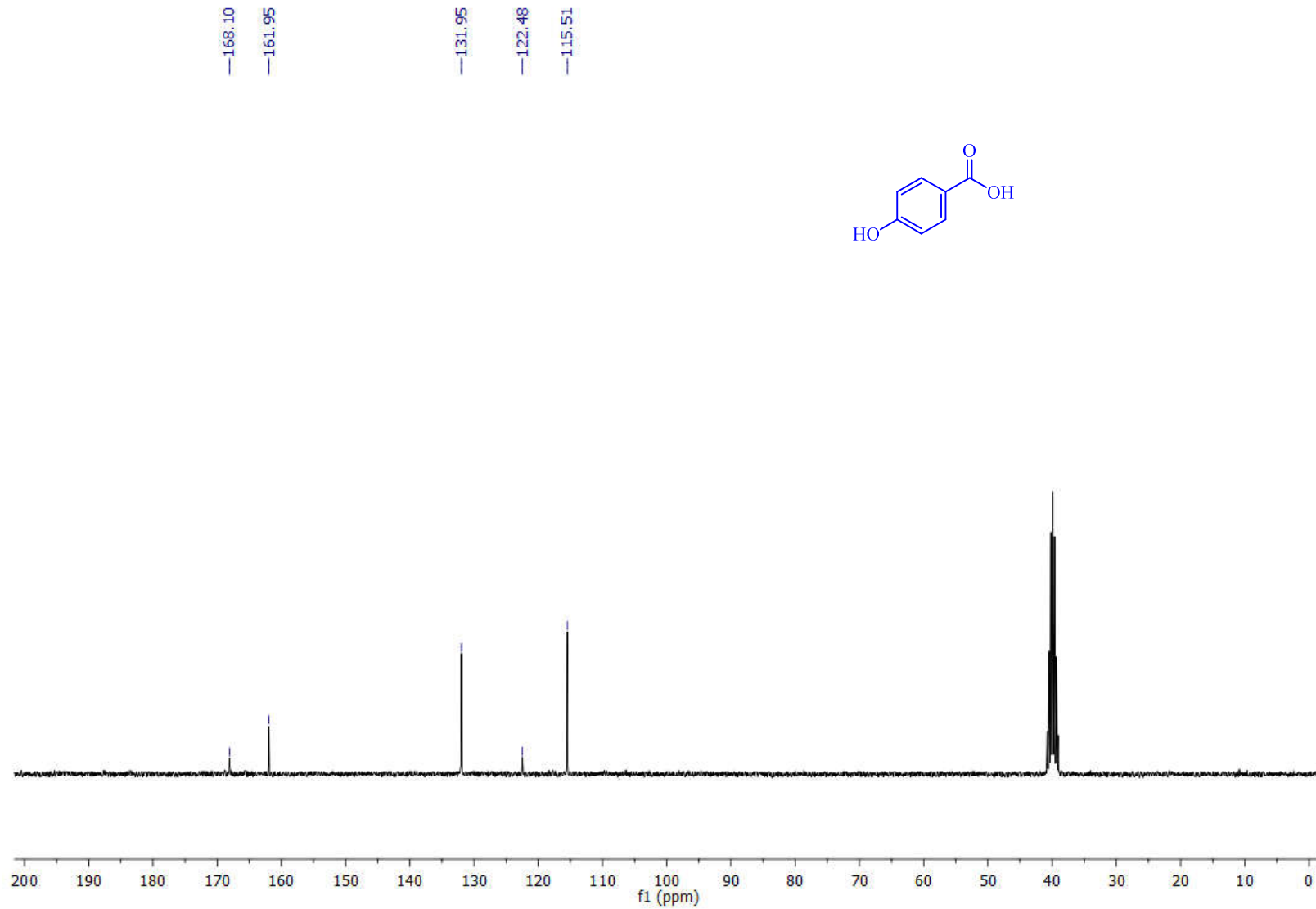


Fig. 11 ^{13}C NMR of 4-hydroxybenzoic acid (**2d**)

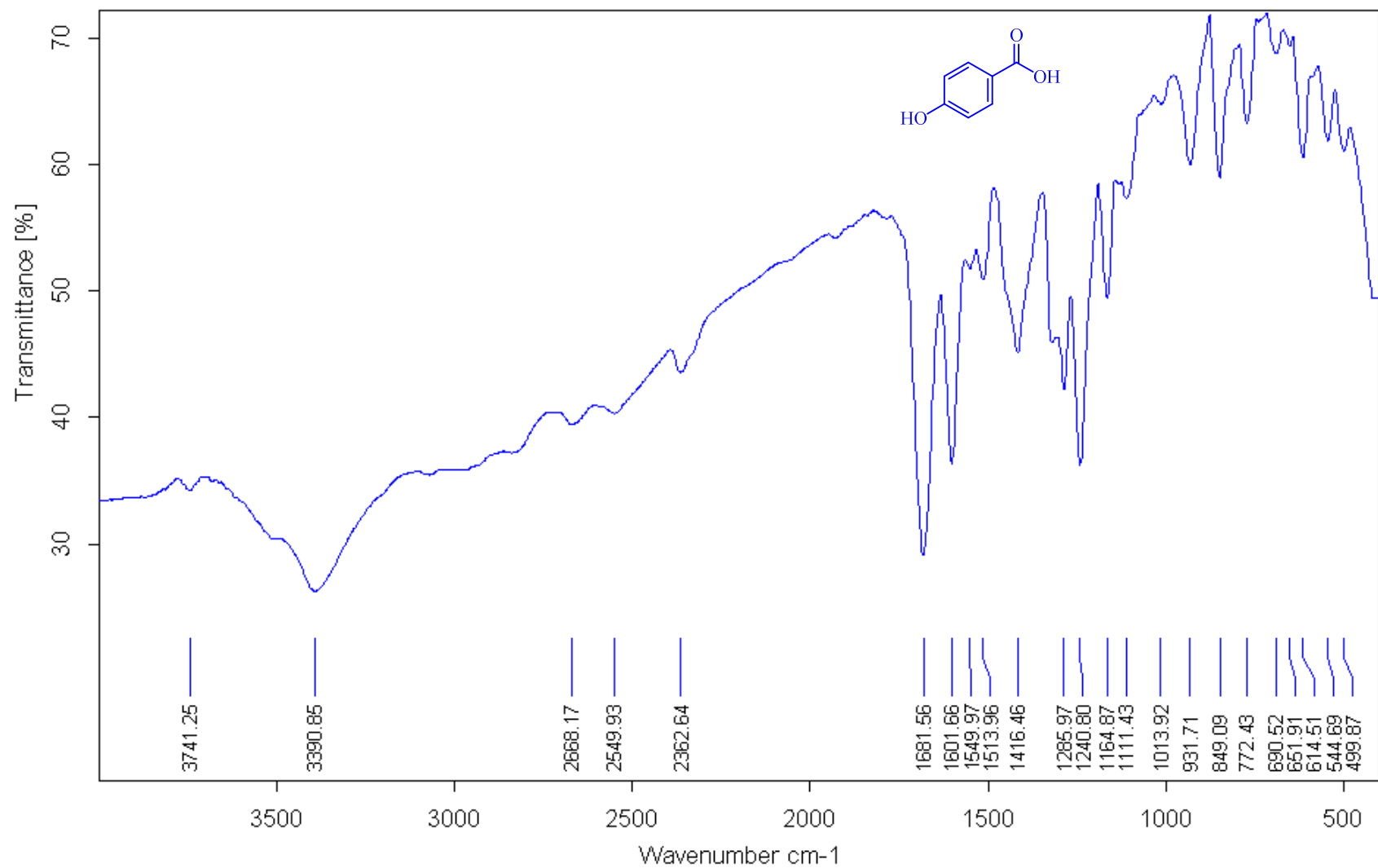


Fig. 12 FT-IR of 4-hydroxybenzoic acid (**2d**)

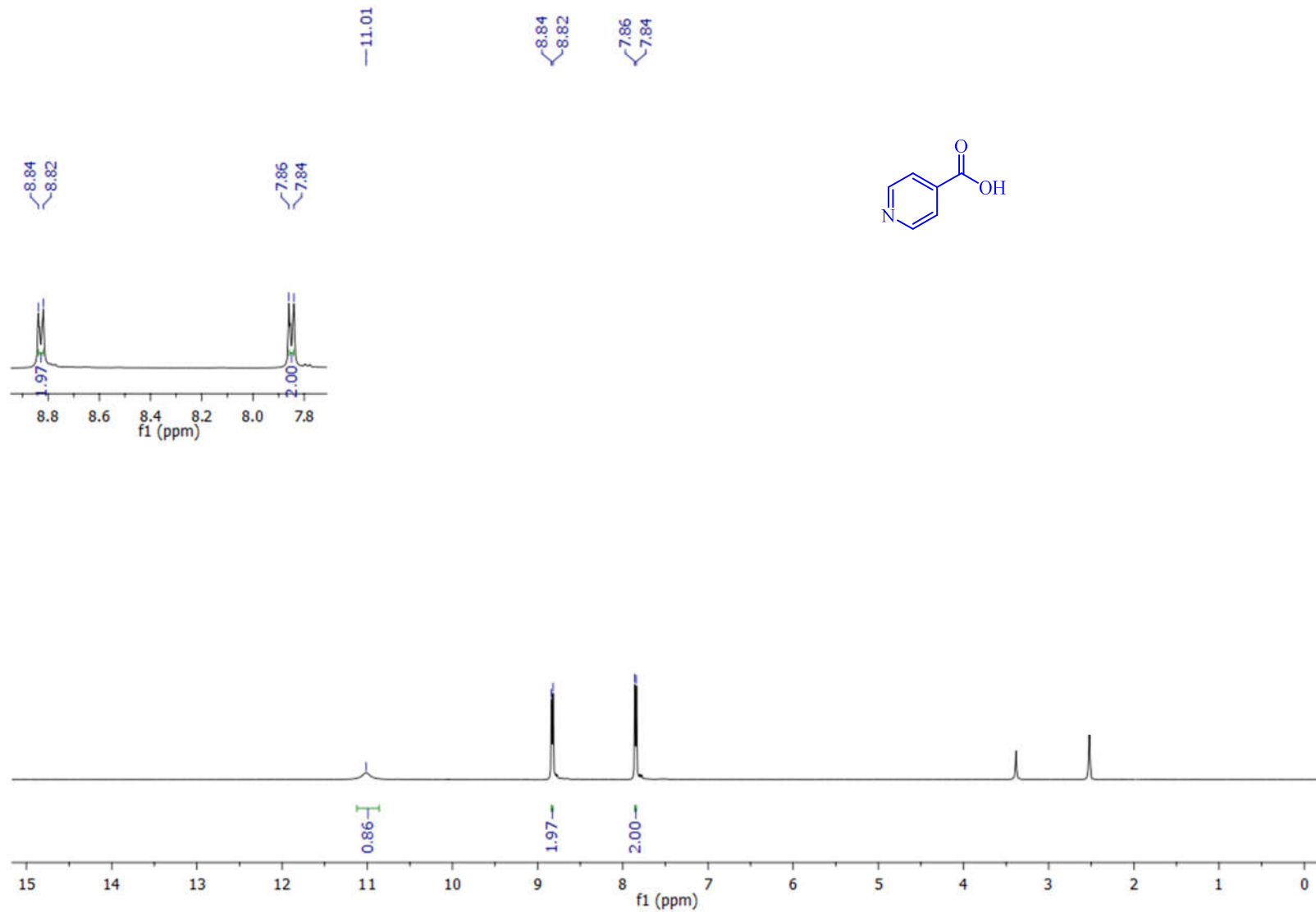


Fig. 13 ^1H NMR of isonicotinic acid (2e)

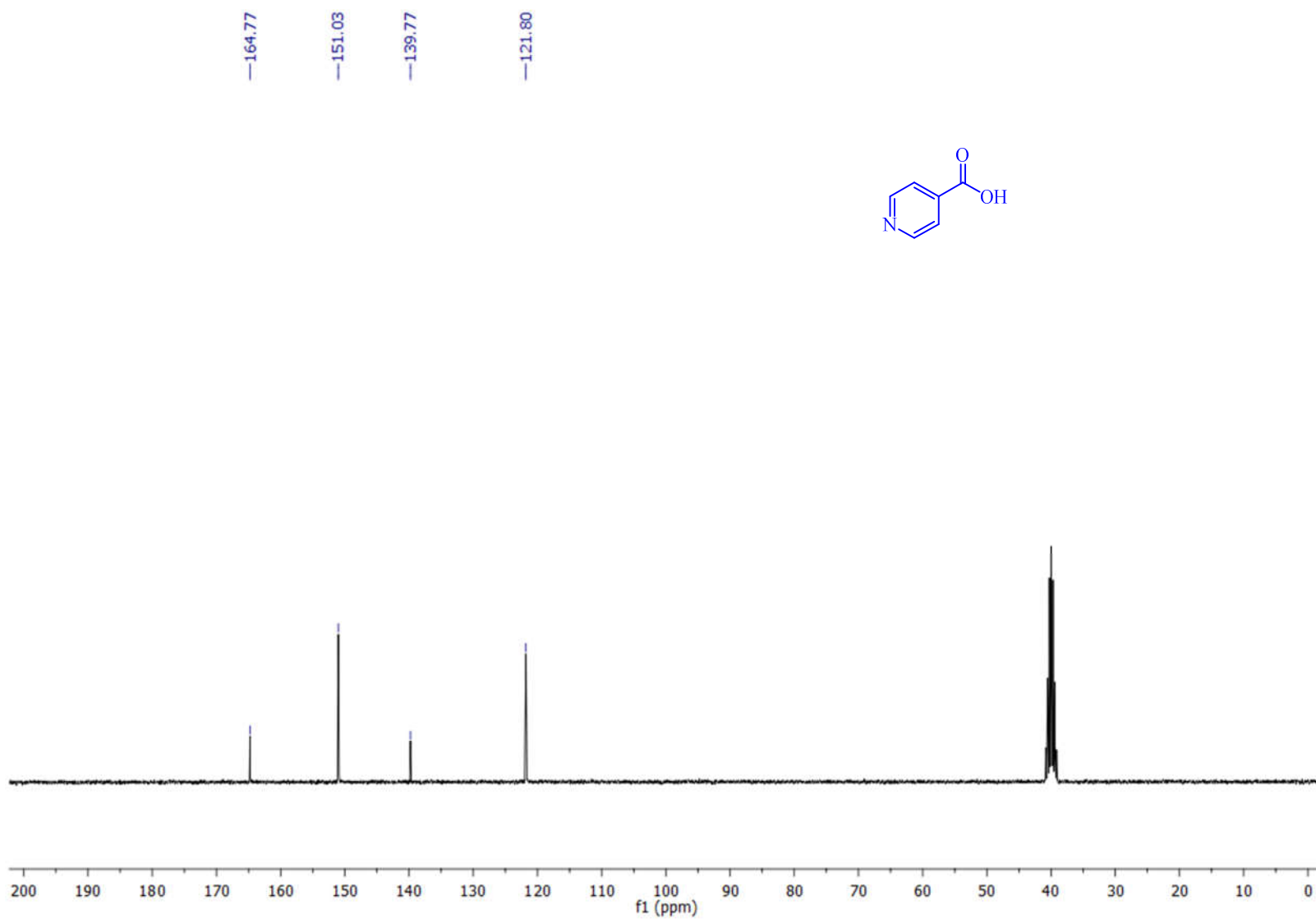


Fig. 14 ^{13}C NMR of isonicotinic acid (**2e**)

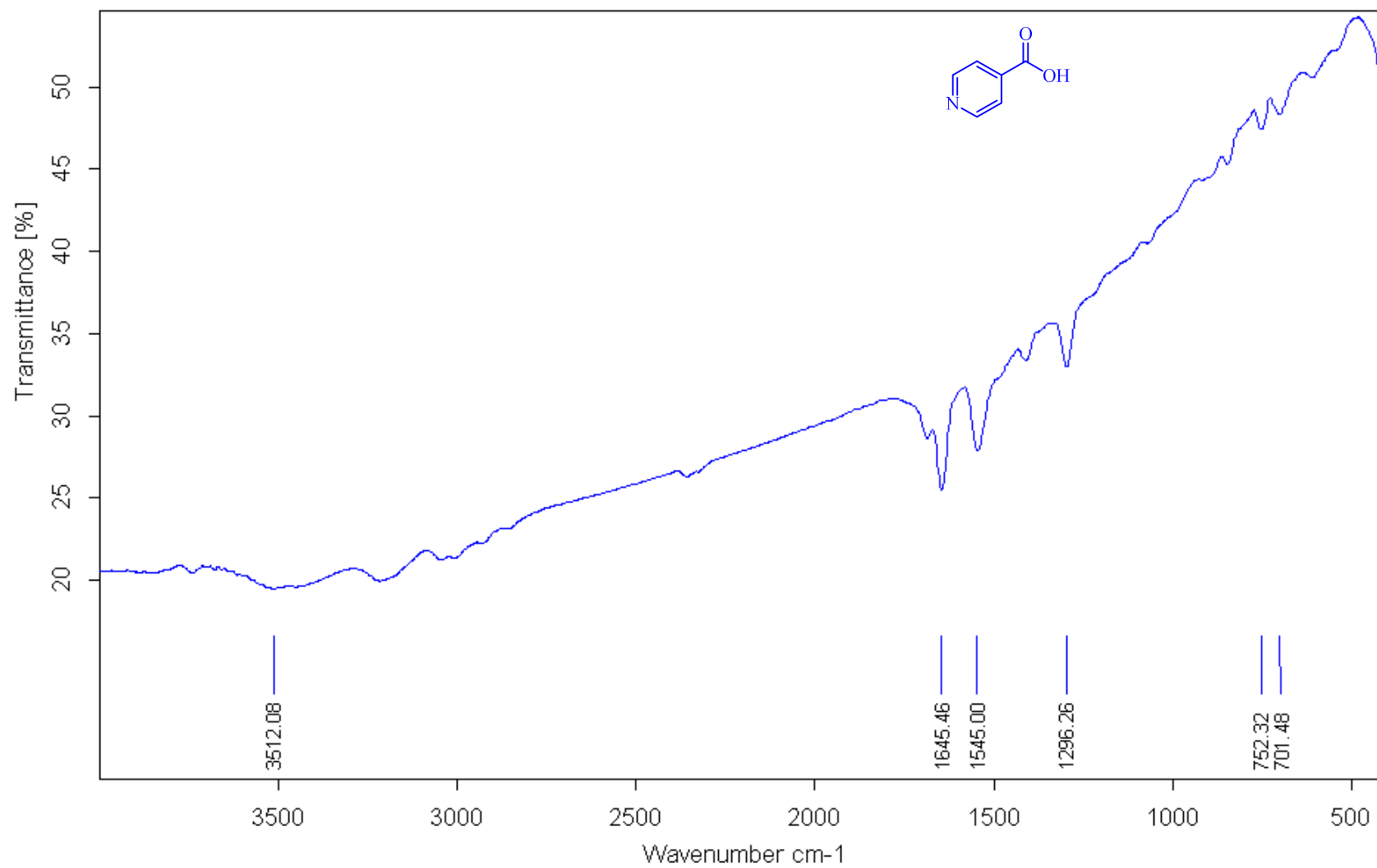


Fig. 15 FT-IR of isonicotinic acid (**2e**)

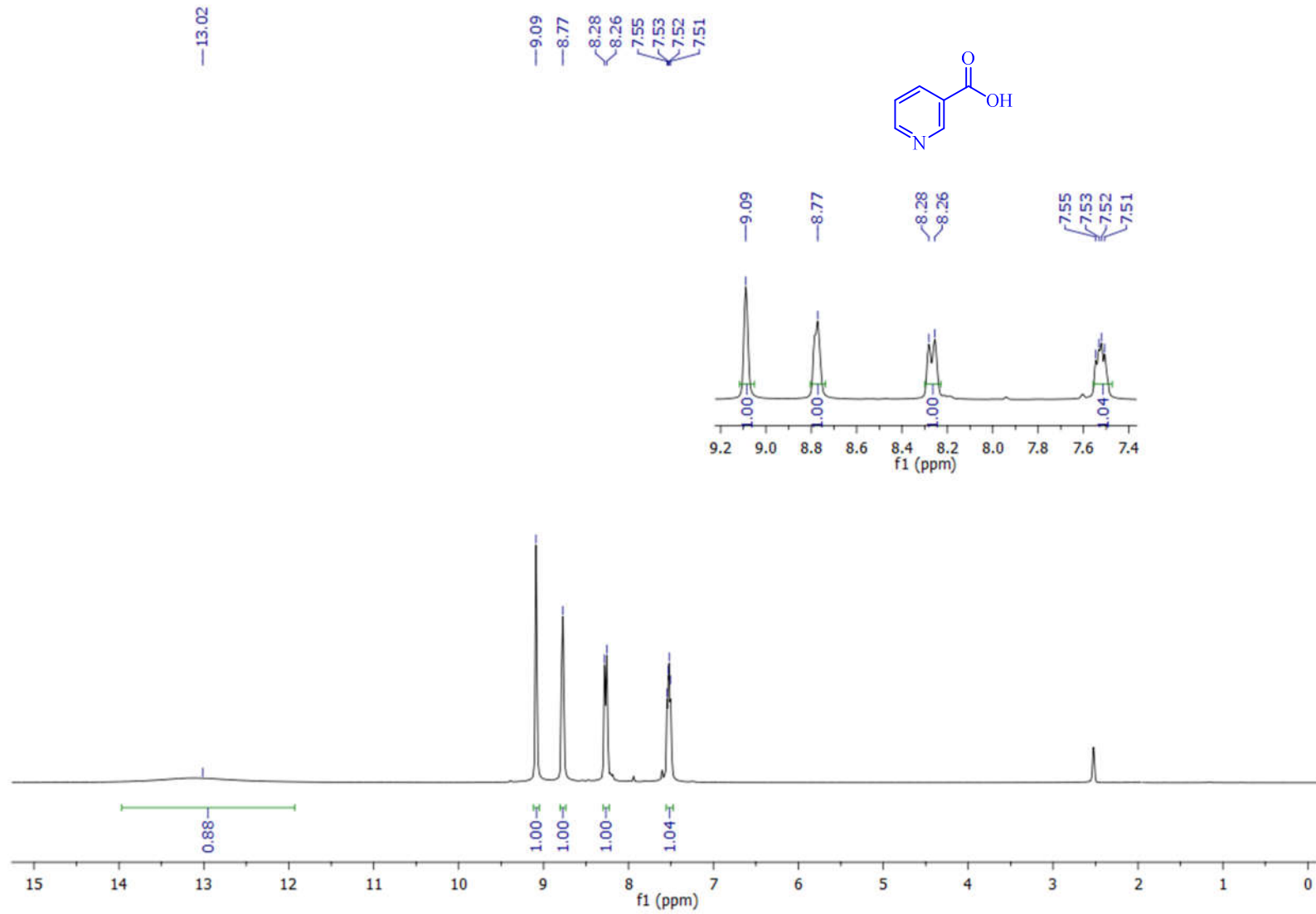


Fig. 16 ^1H NMR of nicotinic acid (**2f**)

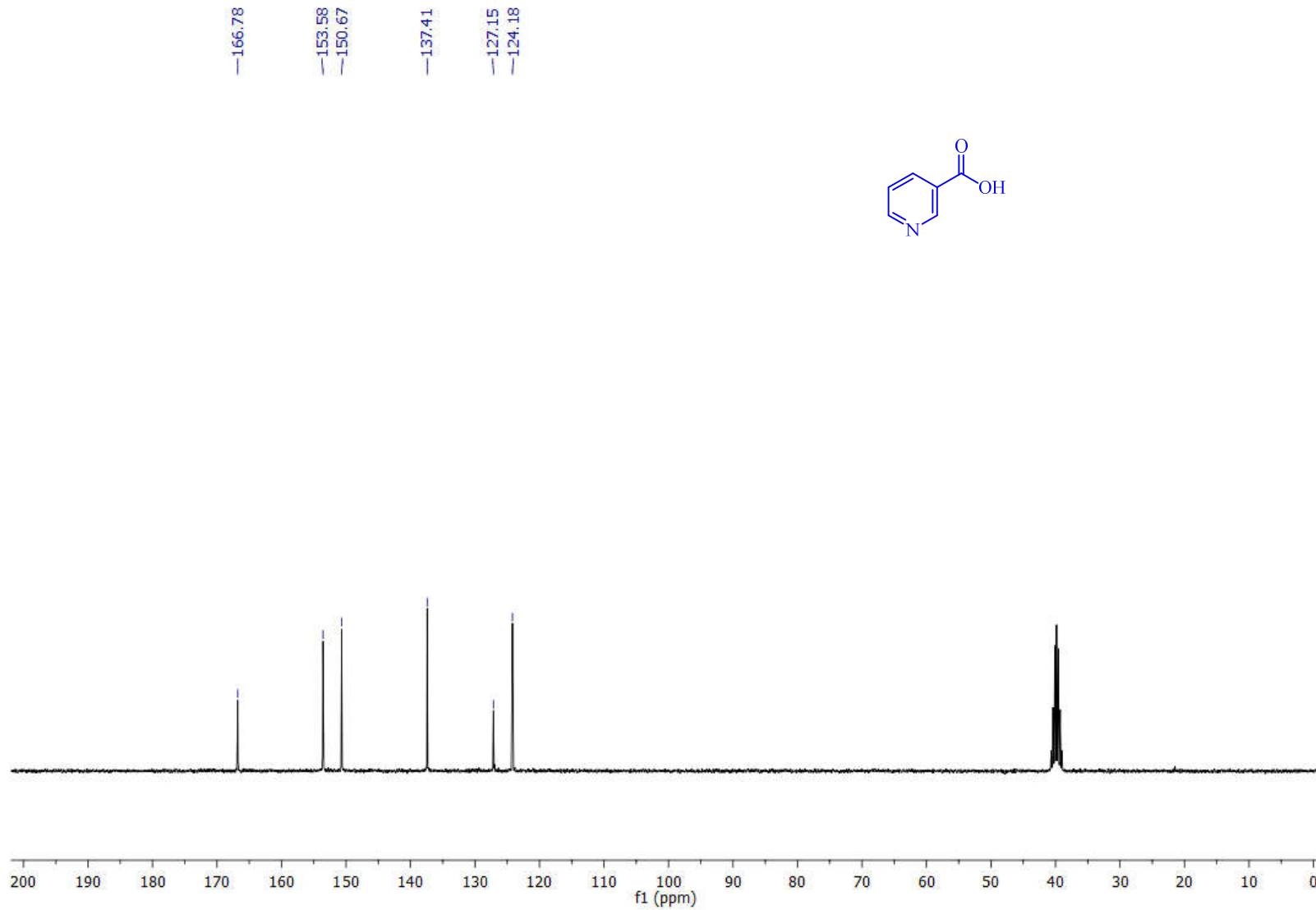


Fig. 17 ^{13}C NMR of nicotinic acid (**2f**)

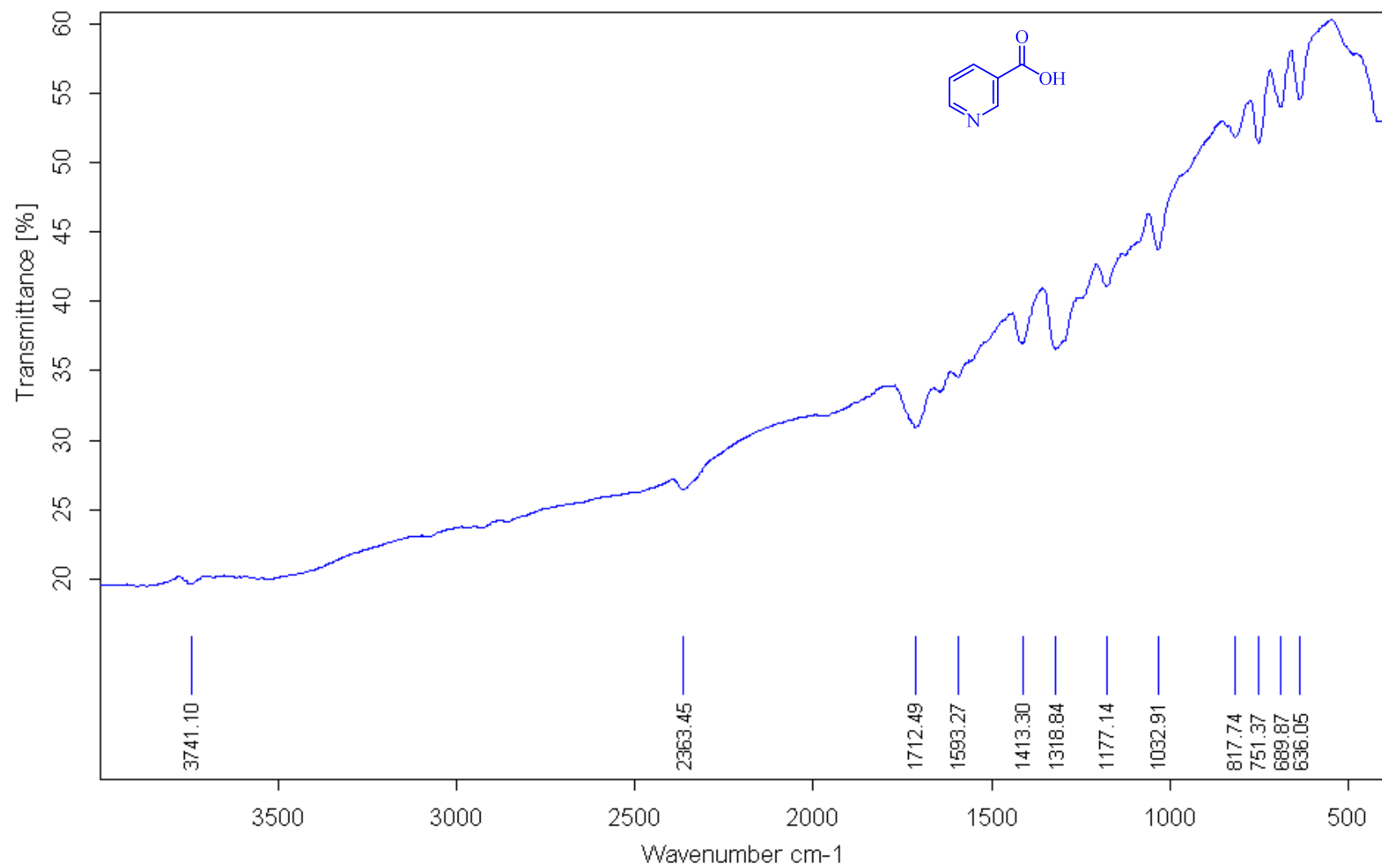


Fig. 18 FT-IR of nicotinic acid (**2f**)

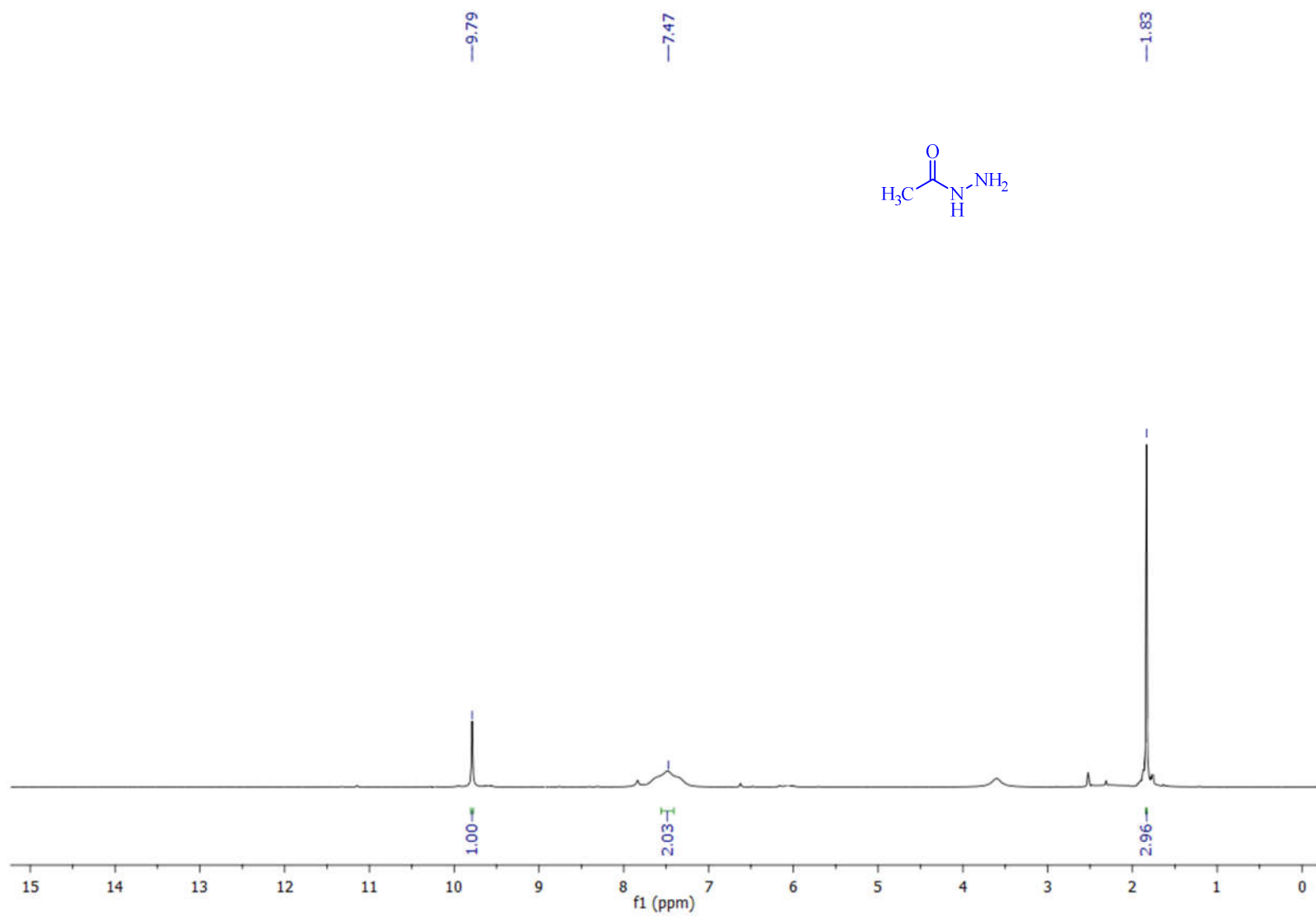


Fig. 19 ¹H NMR of acetohydrazide (**2g**)

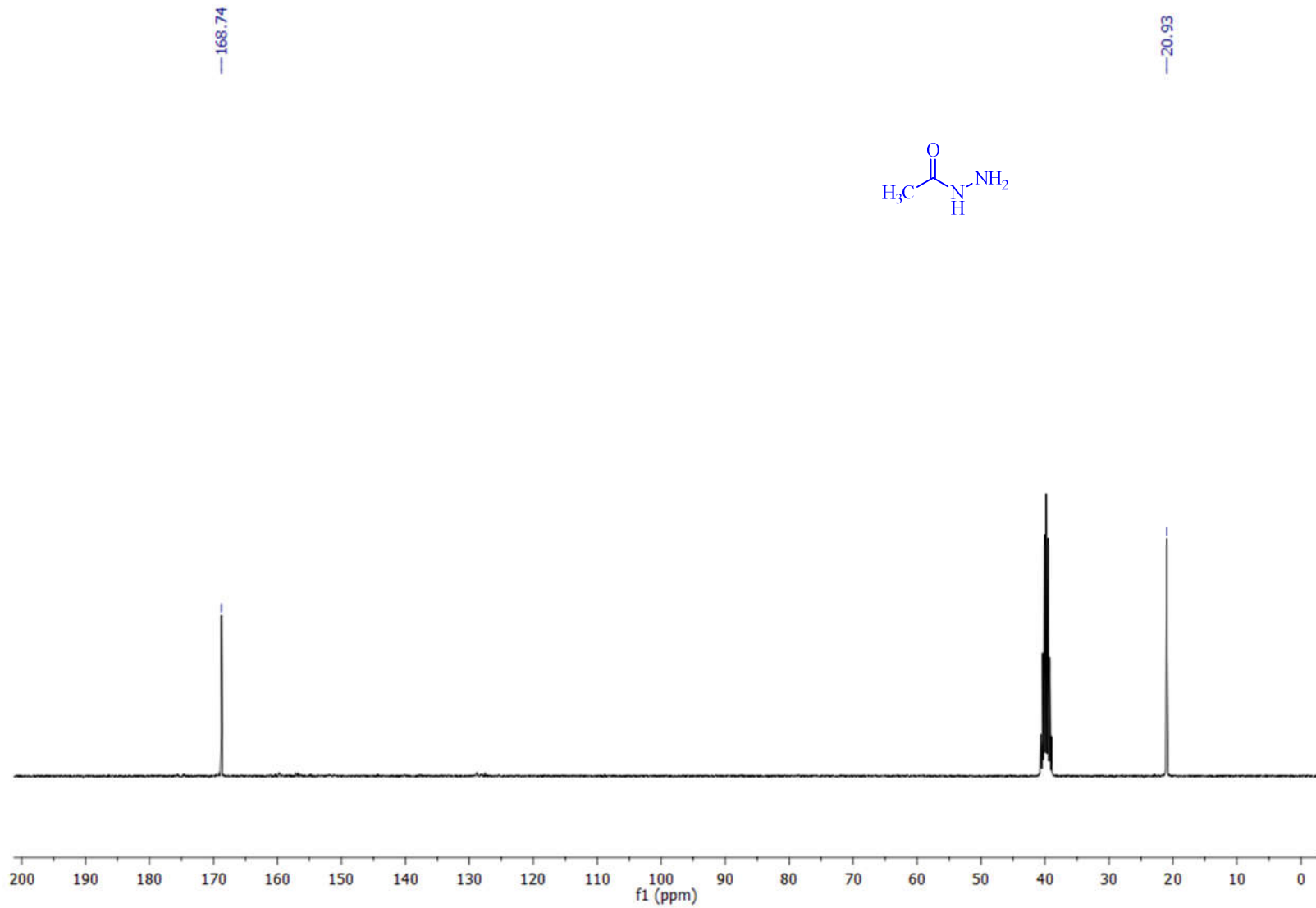


Fig. 20 ^{13}C NMR of acetohydrazide (**2g**)

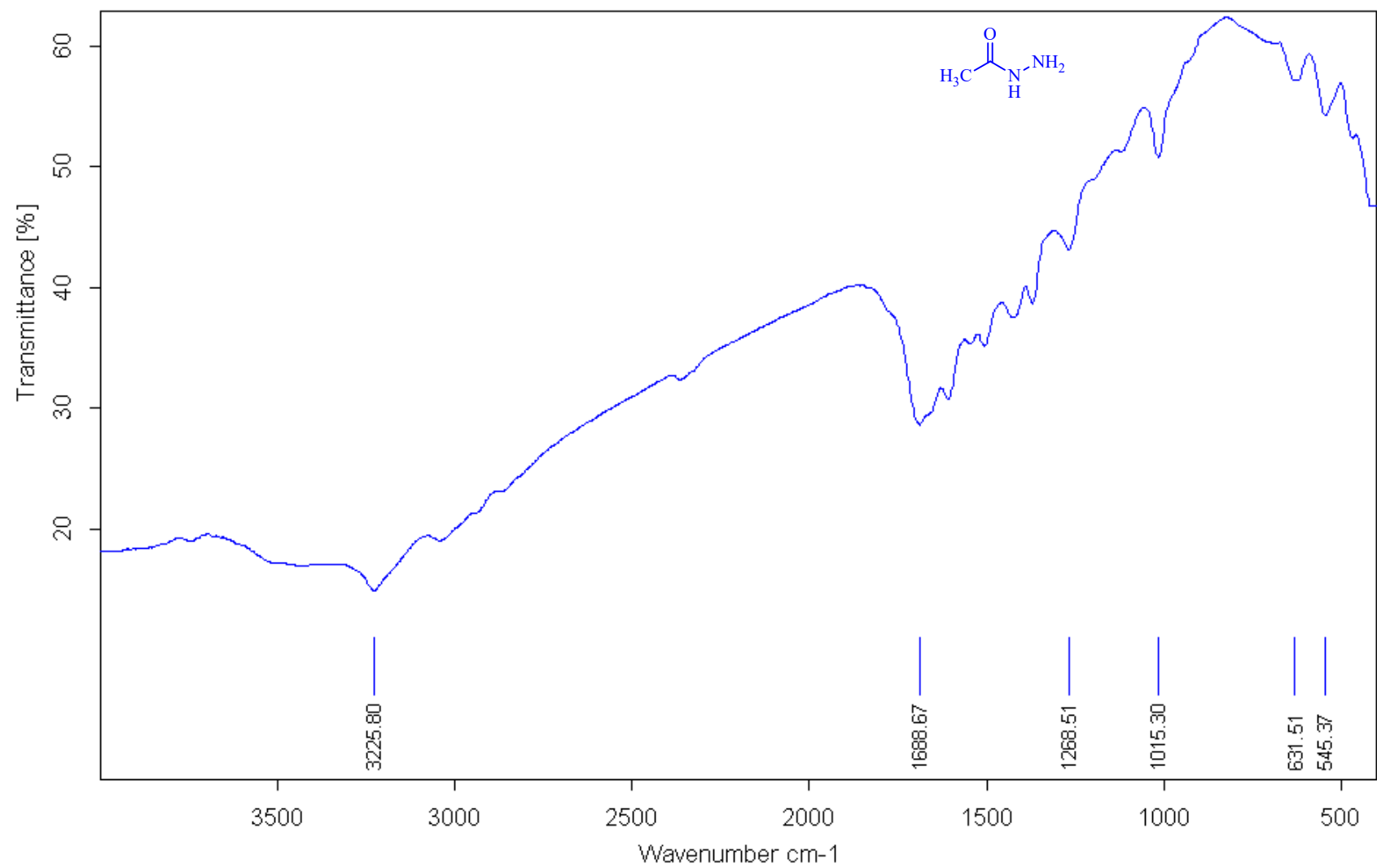


Fig. 21 FT-IR of acetohydrazide (**2g**)

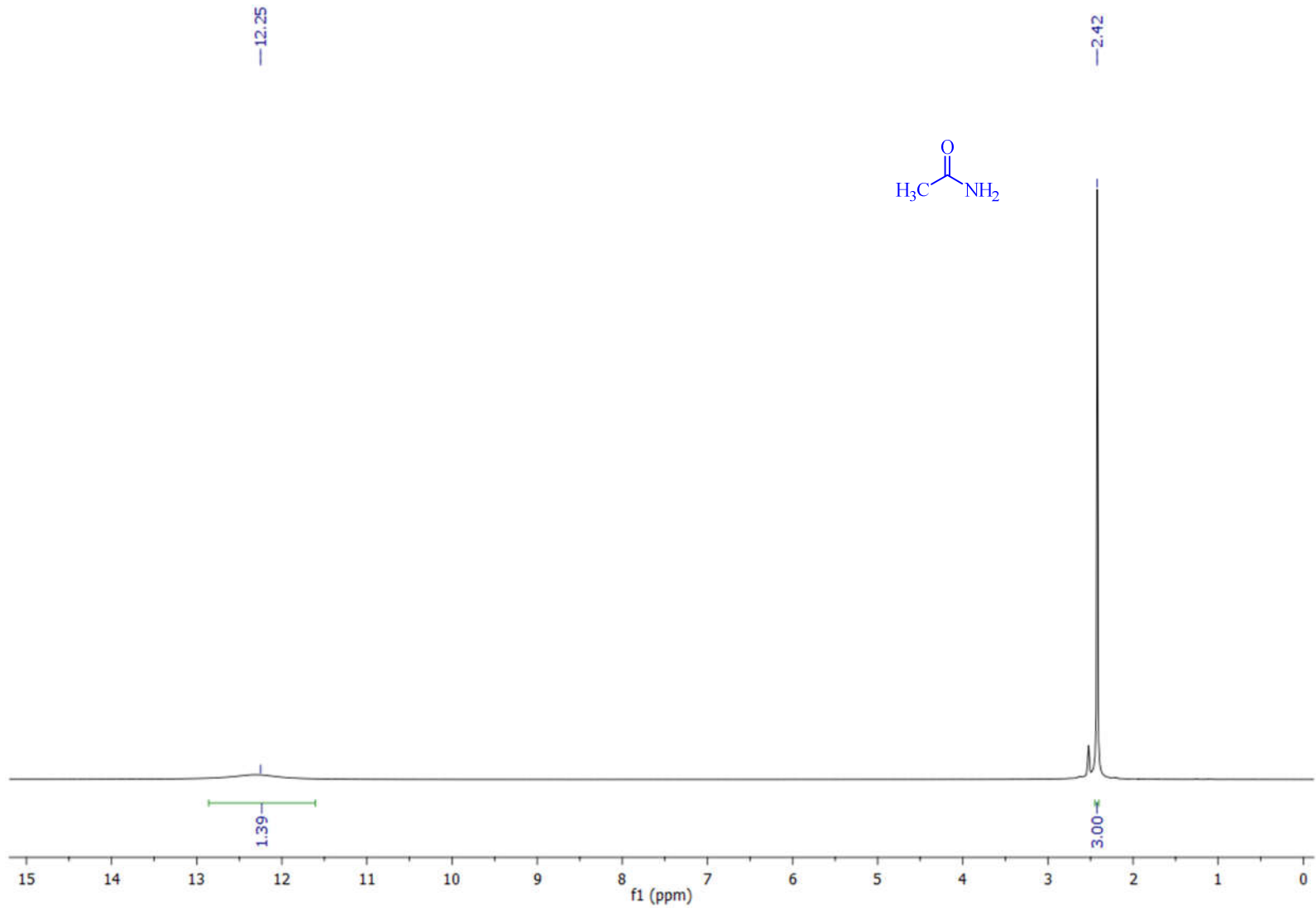


Fig. 22 ^1H NMR of acetamide (**2h**)

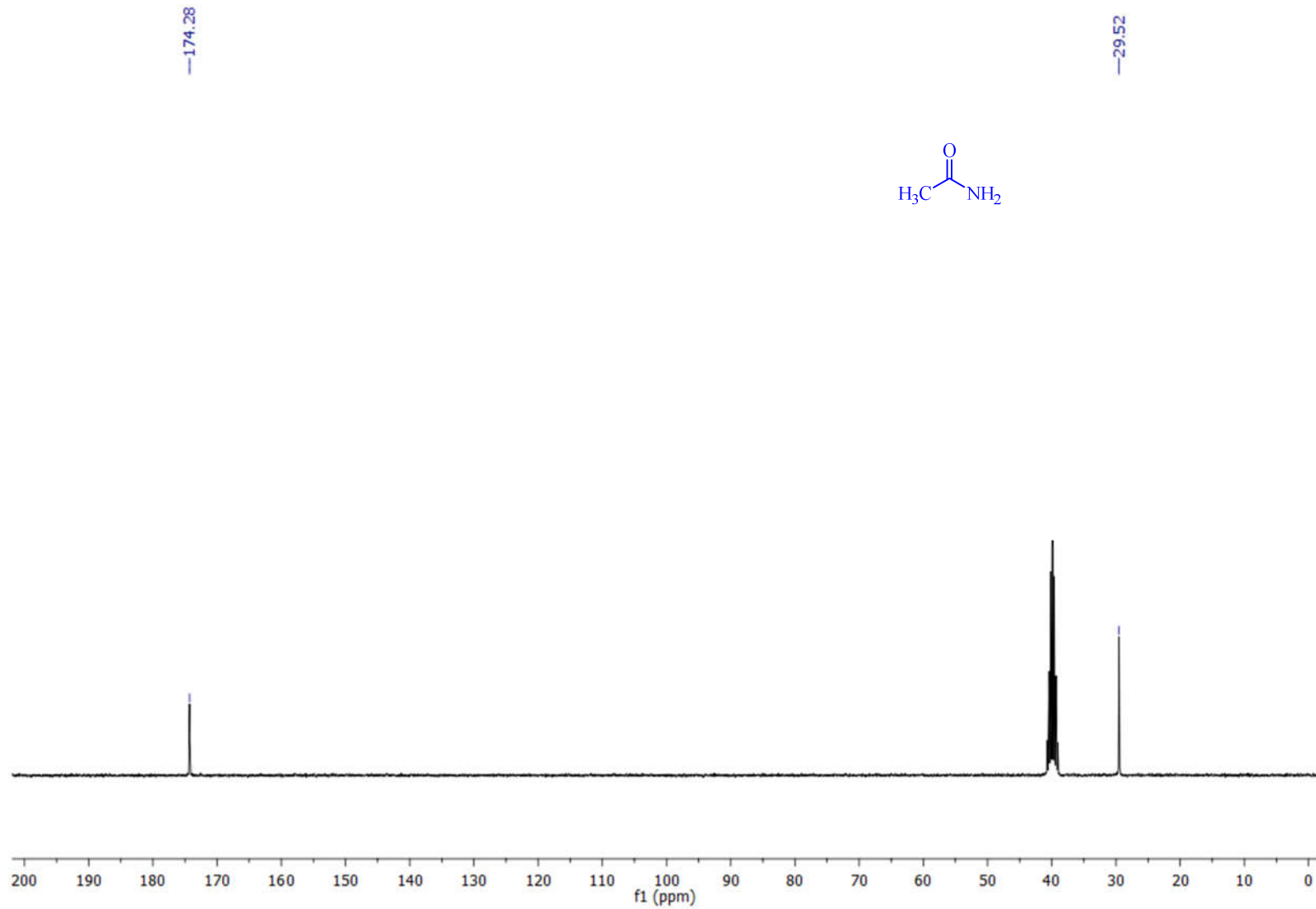


Fig. 23 ^{13}C NMR of acetamide (**2h**)

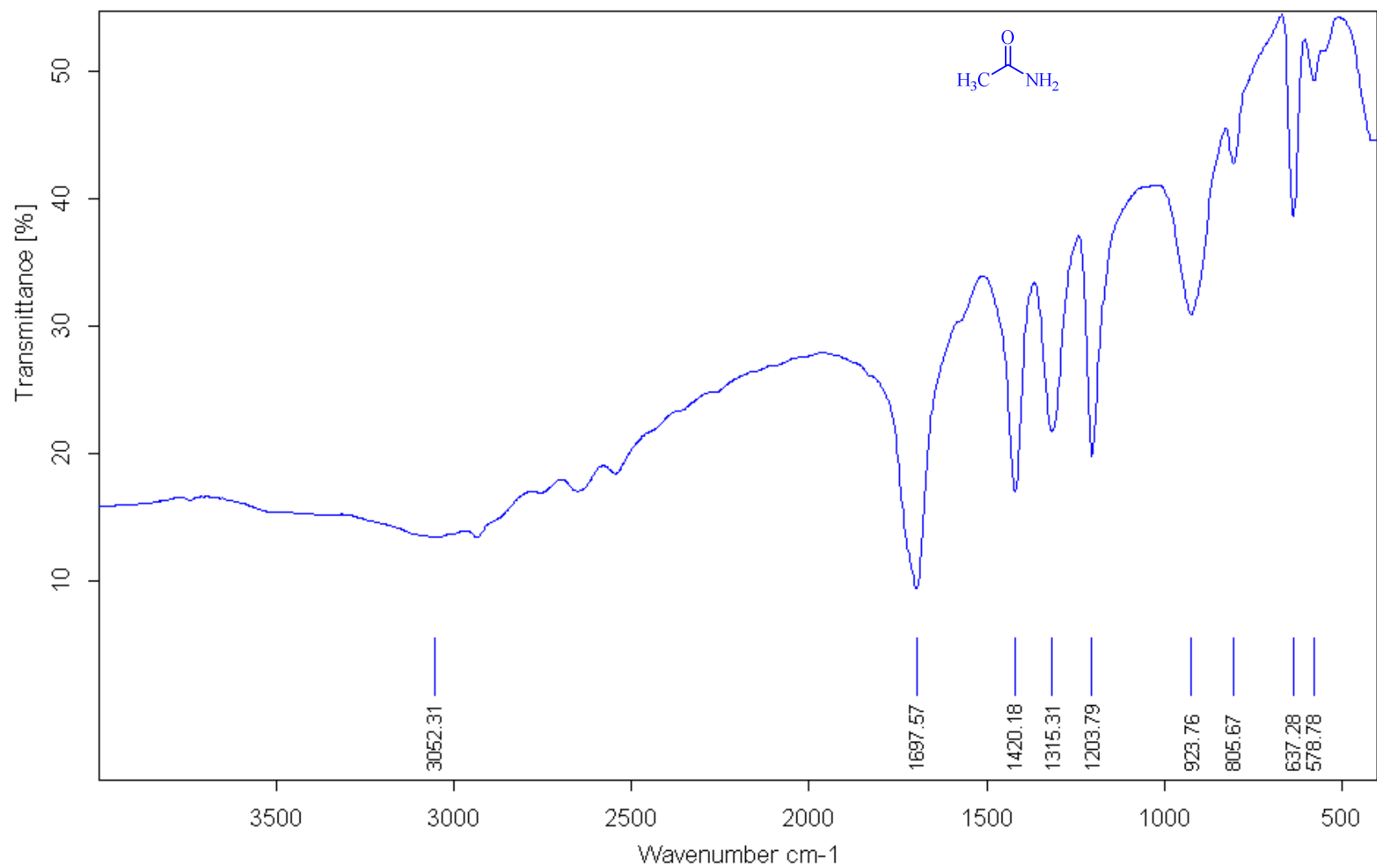


Fig. 24 FT-IR of acetamide (**2h**)

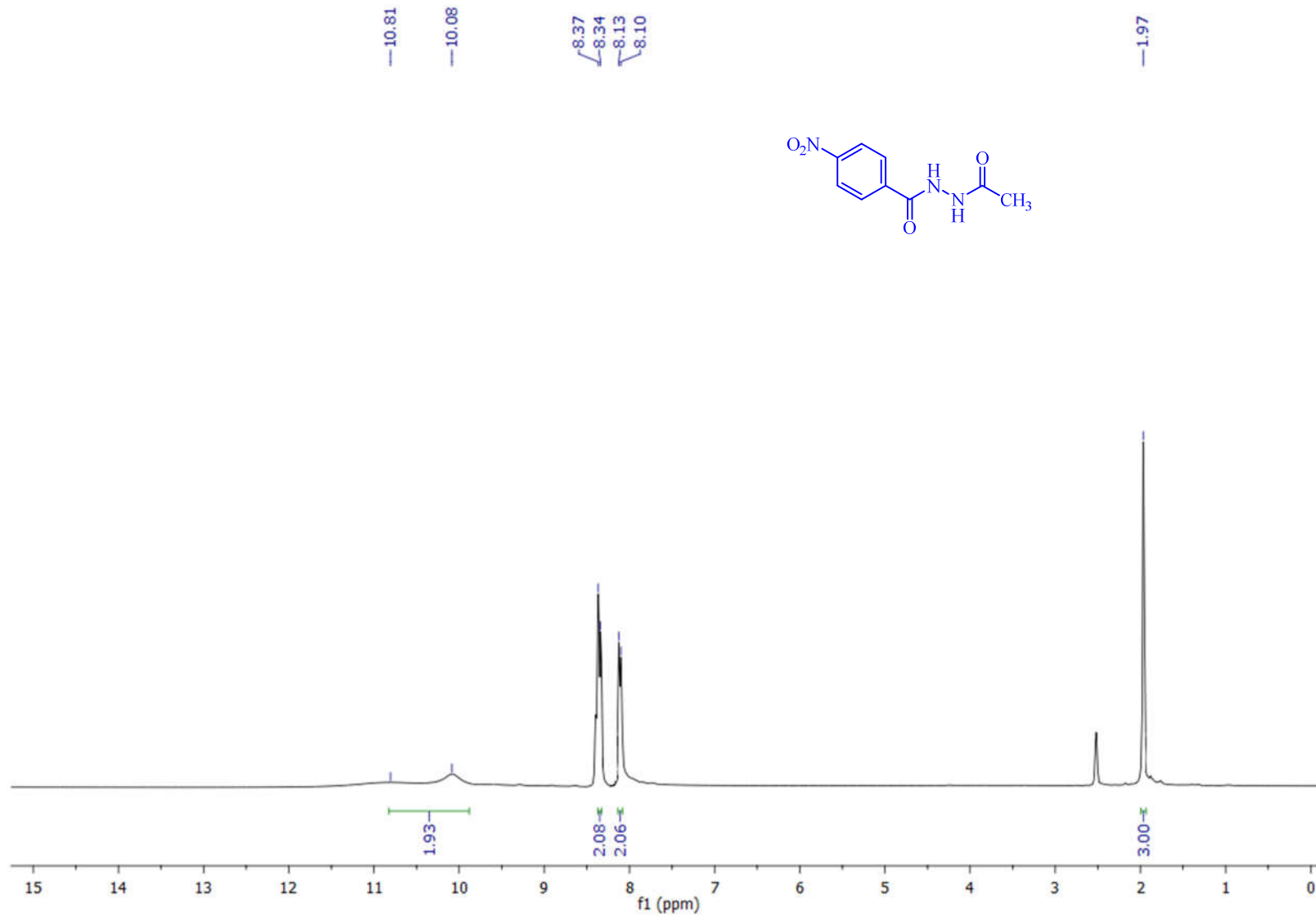


Fig. 25 ^1H NMR of *N'*-acetyl-4-nitrobenzohydrazide (**2i**)

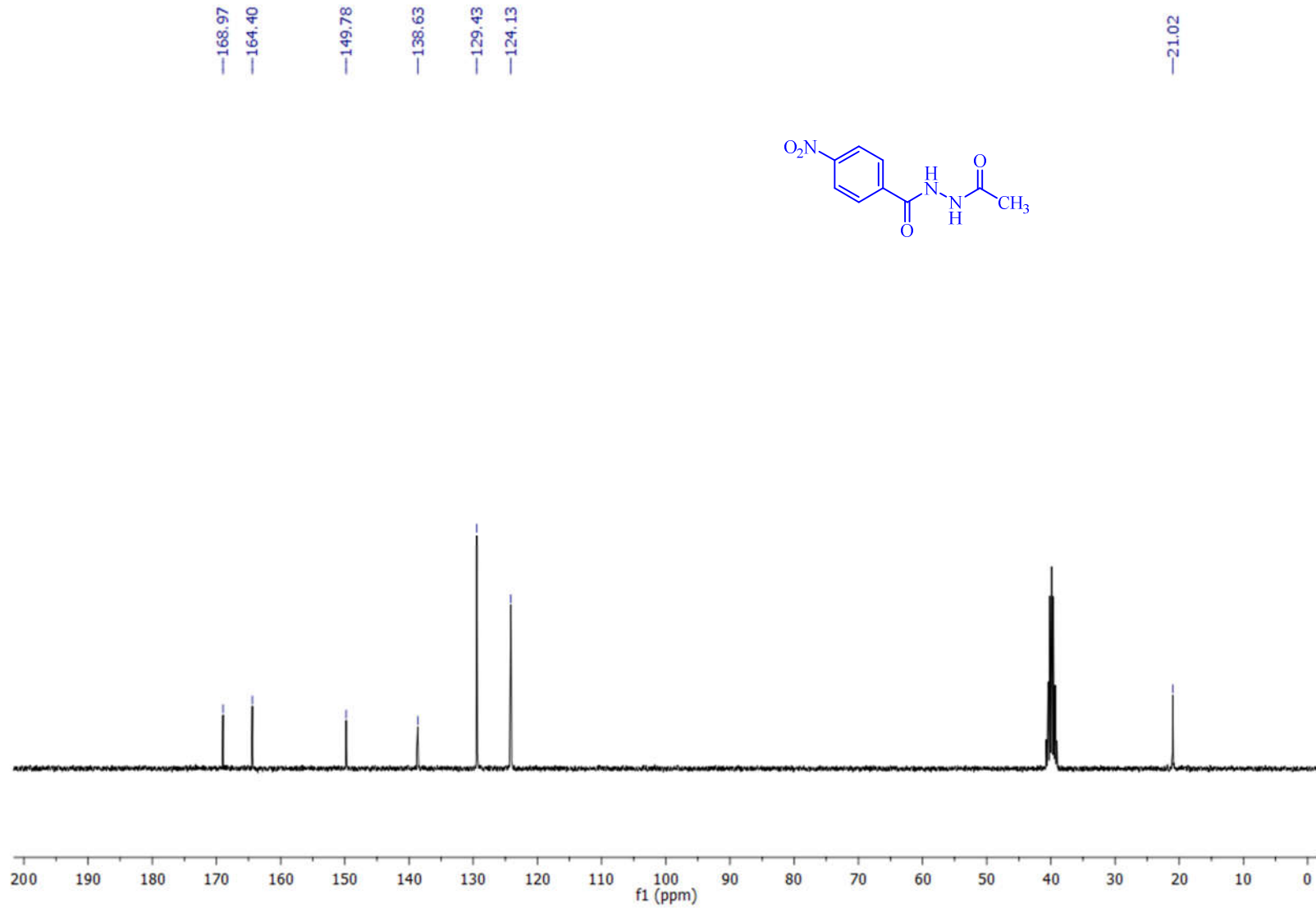


Fig. 26 ^{13}C NMR of *N'*-acetyl-4-nitrobenzohydrazide (**2i**)

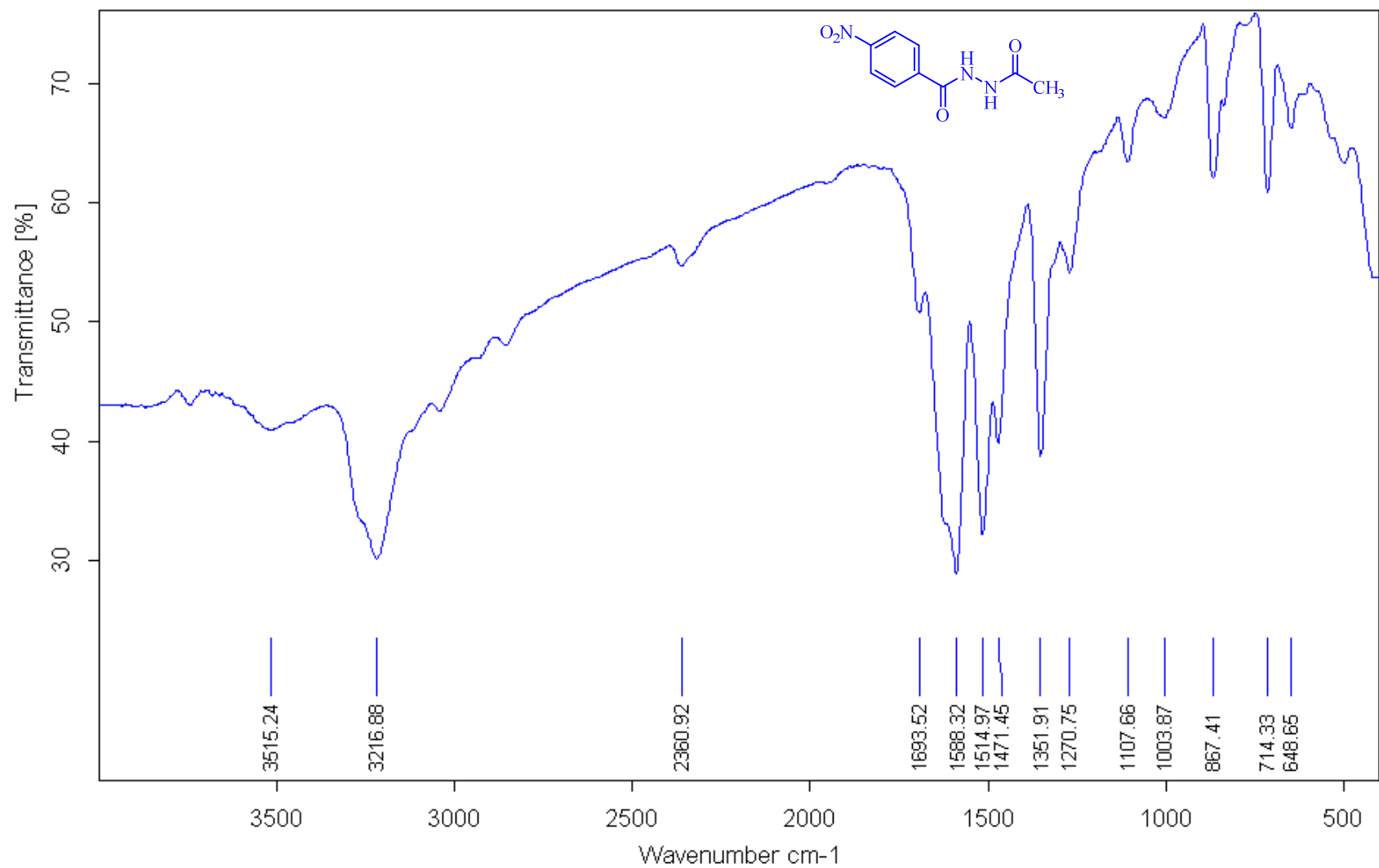


Fig. 27 FT-IR of *N'*-acetyl-4-nitrobenzohydrazide (**2i**)

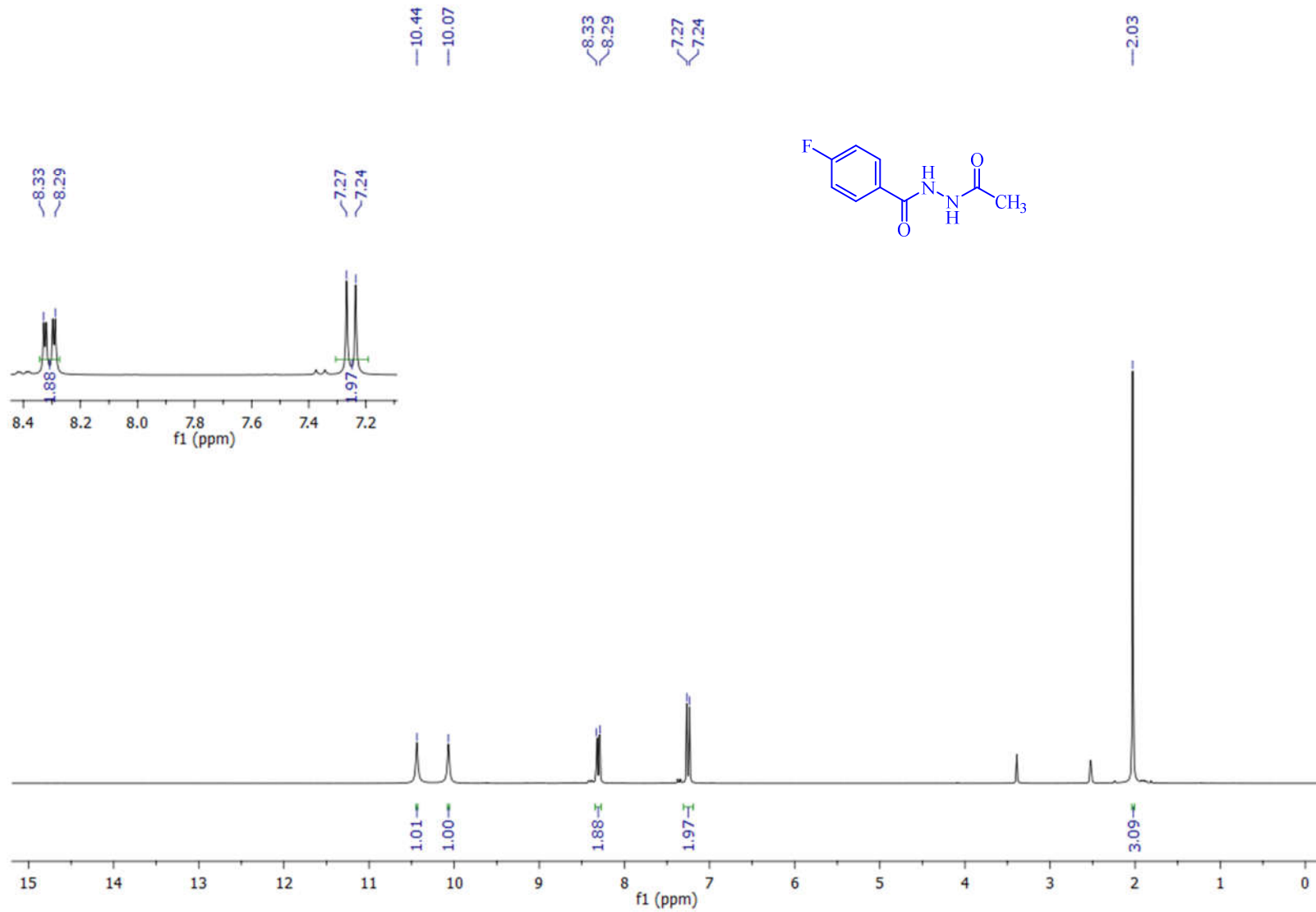


Fig. 28 ¹H NMR of *N'*-acetyl-4-fluorobenzohydrazide (**2j**)

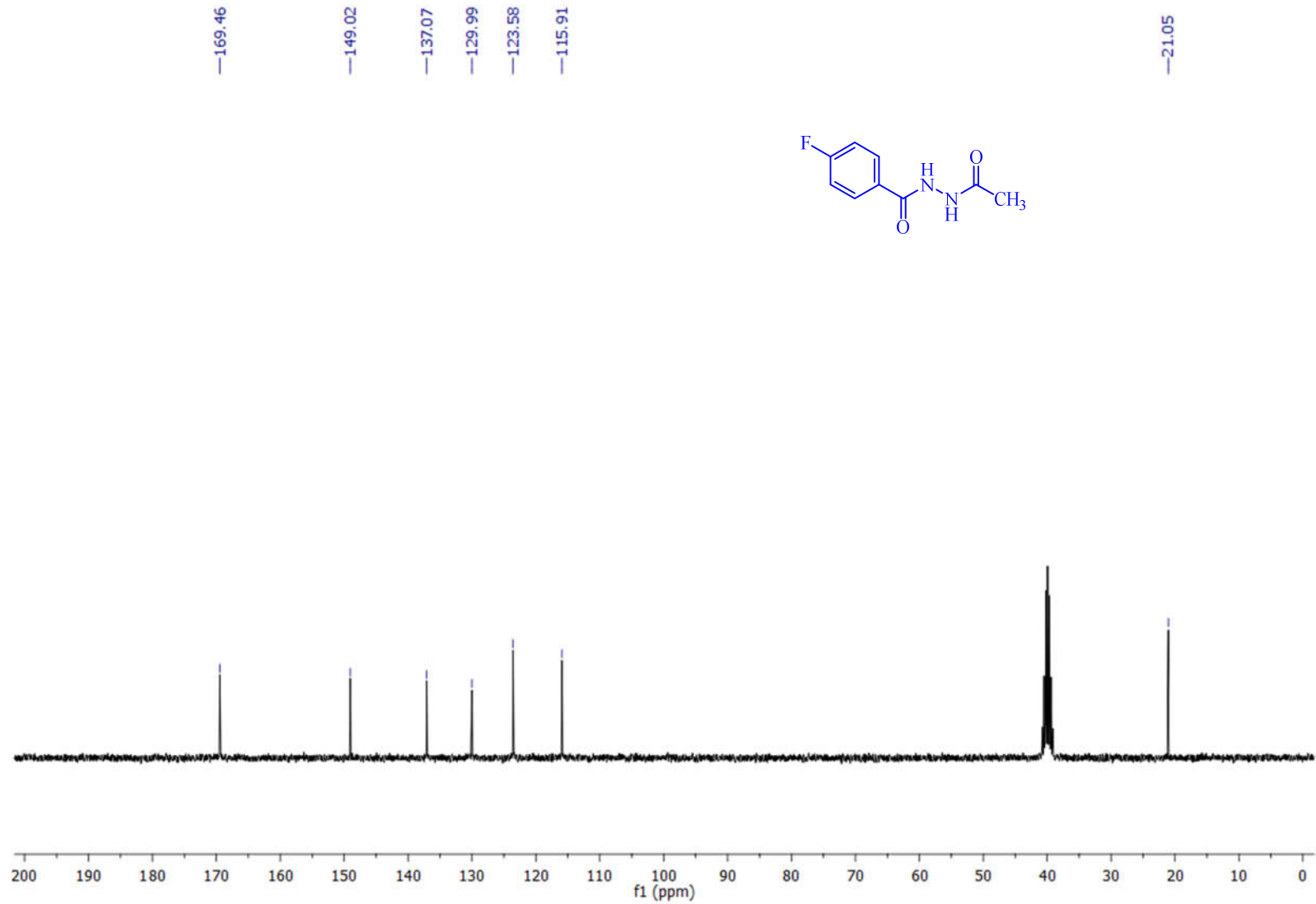


Fig. 29 ^{13}C NMR of *N'*-acetyl-4-fluorobenzohydrazide (2j)

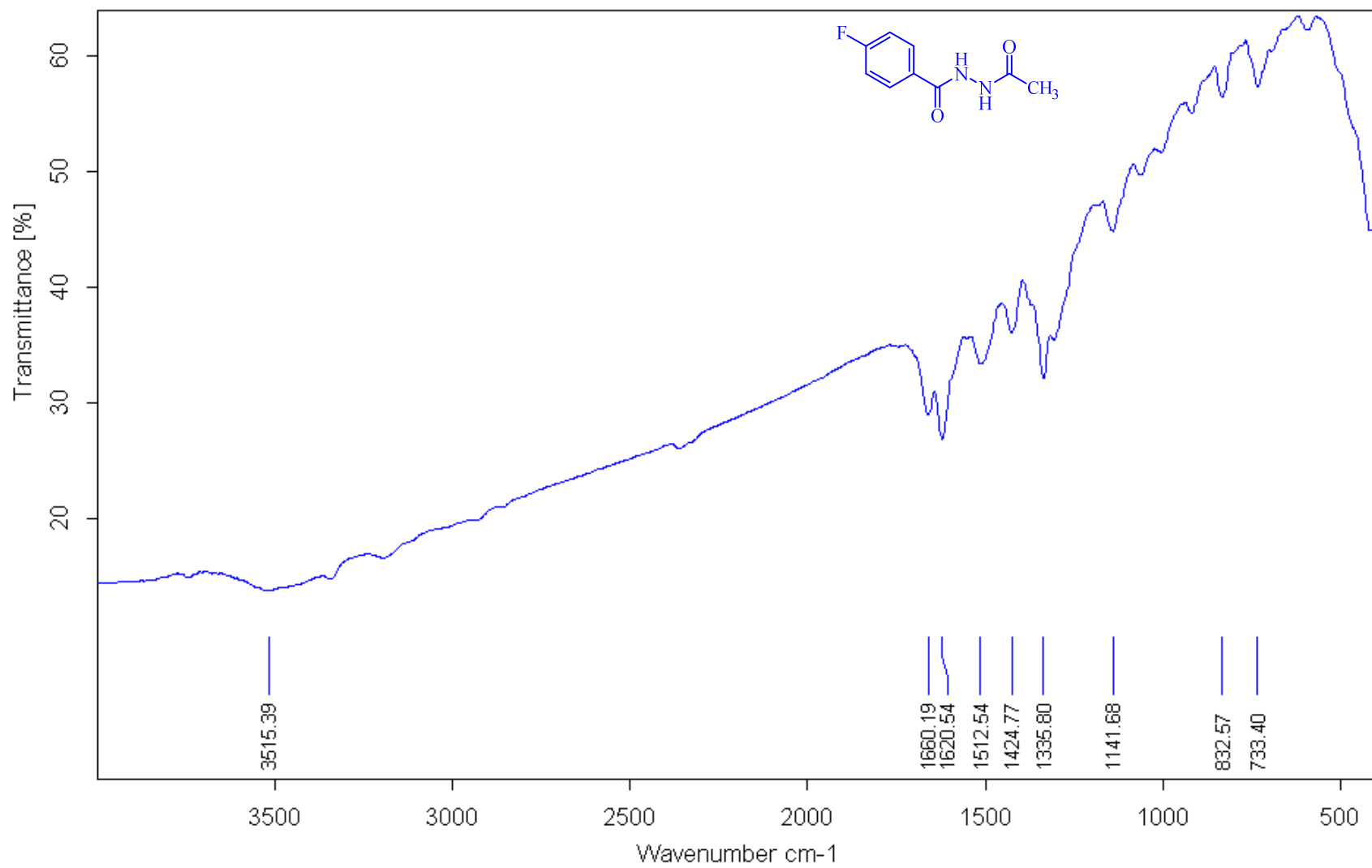


Fig. 30 FT-IR of *N'*-acetyl-4-fluorobenzohydrazide (**2j**)

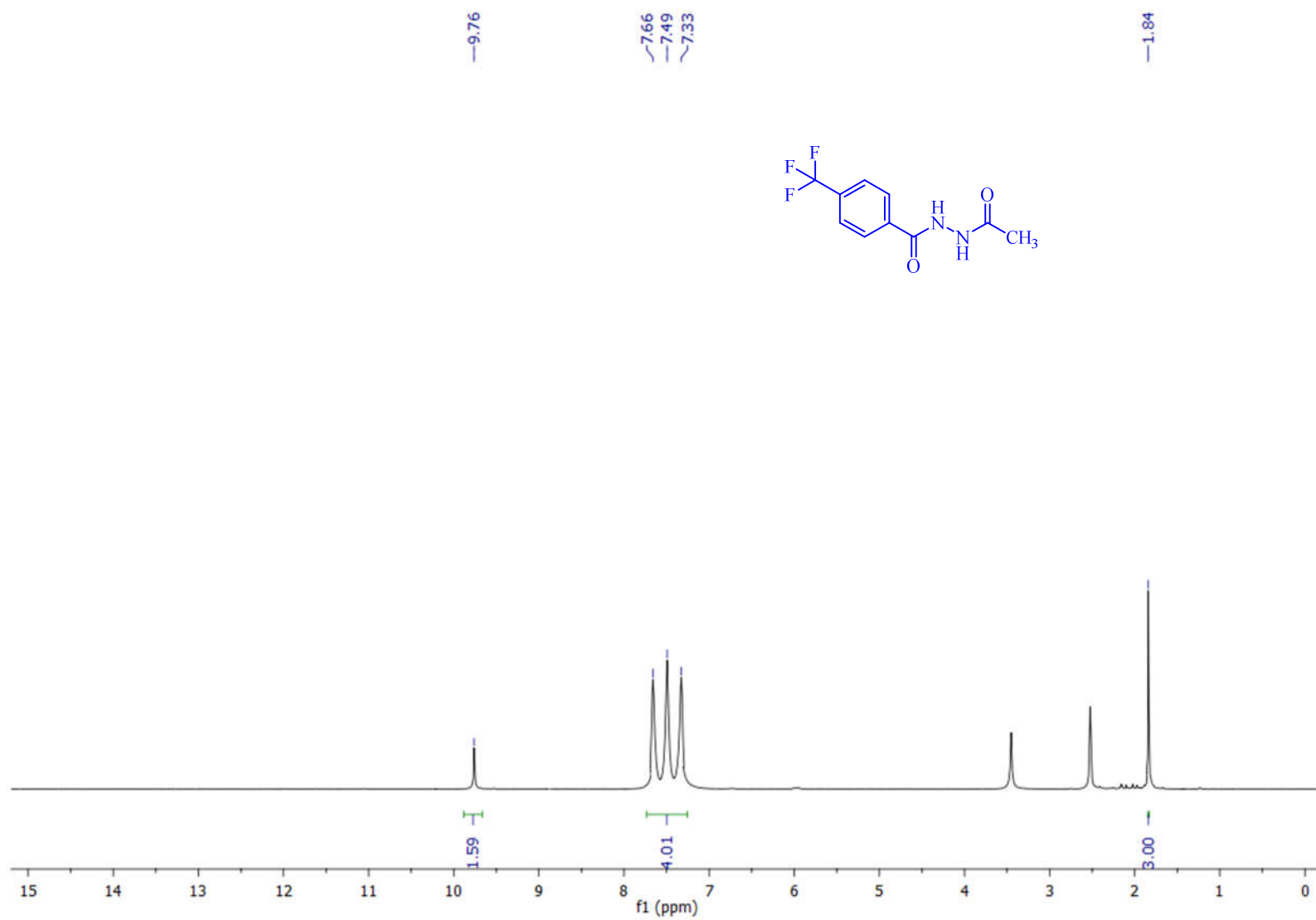


Fig. 31 ¹H NMR of *N'*-acetyl-4-(trifluoromethyl)benzohydrazide (**2k**)

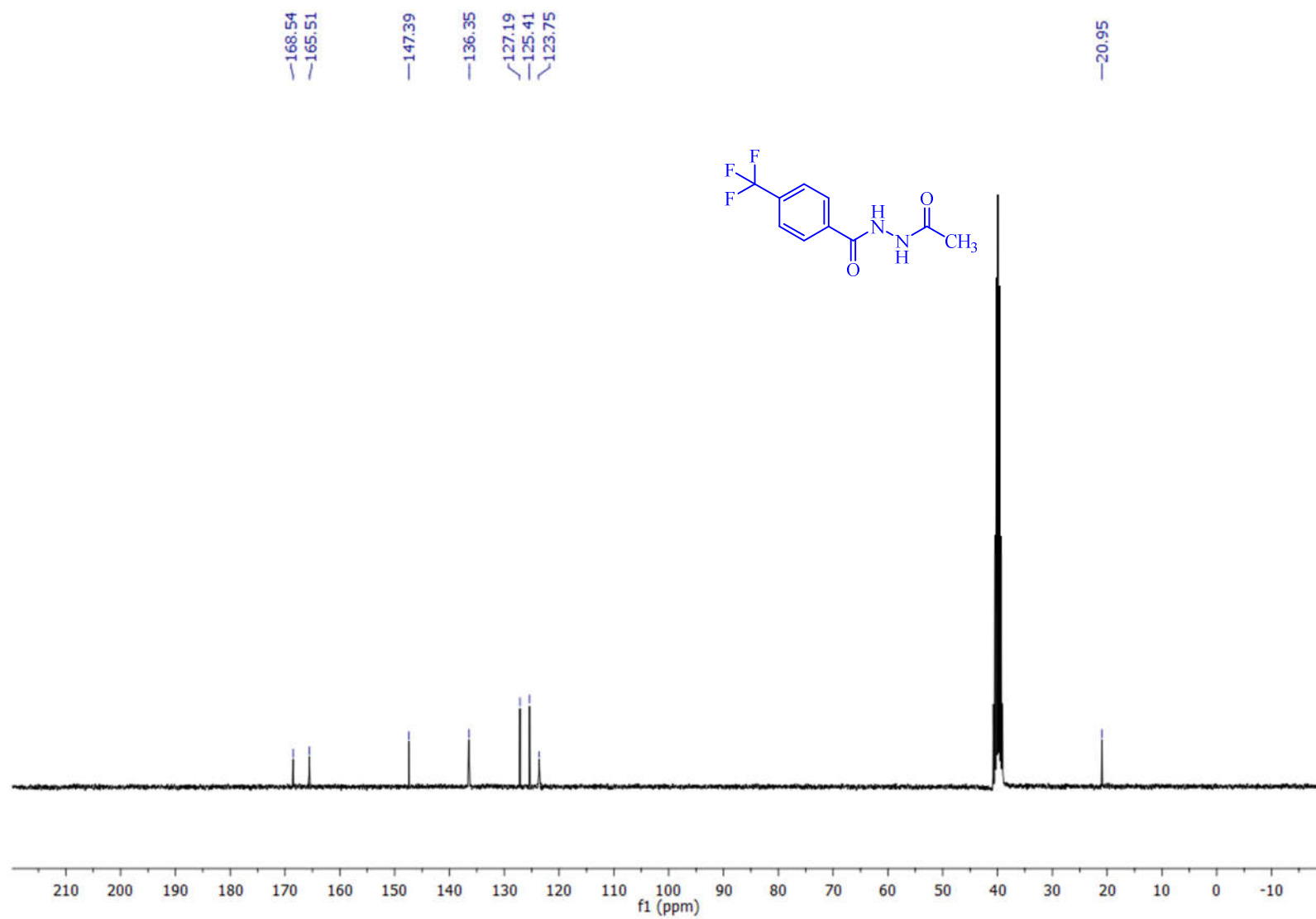


Fig. 32 ^{13}C NMR of *N'*-acetyl-4-(trifluoromethyl)benzohydrazide (**2k**)

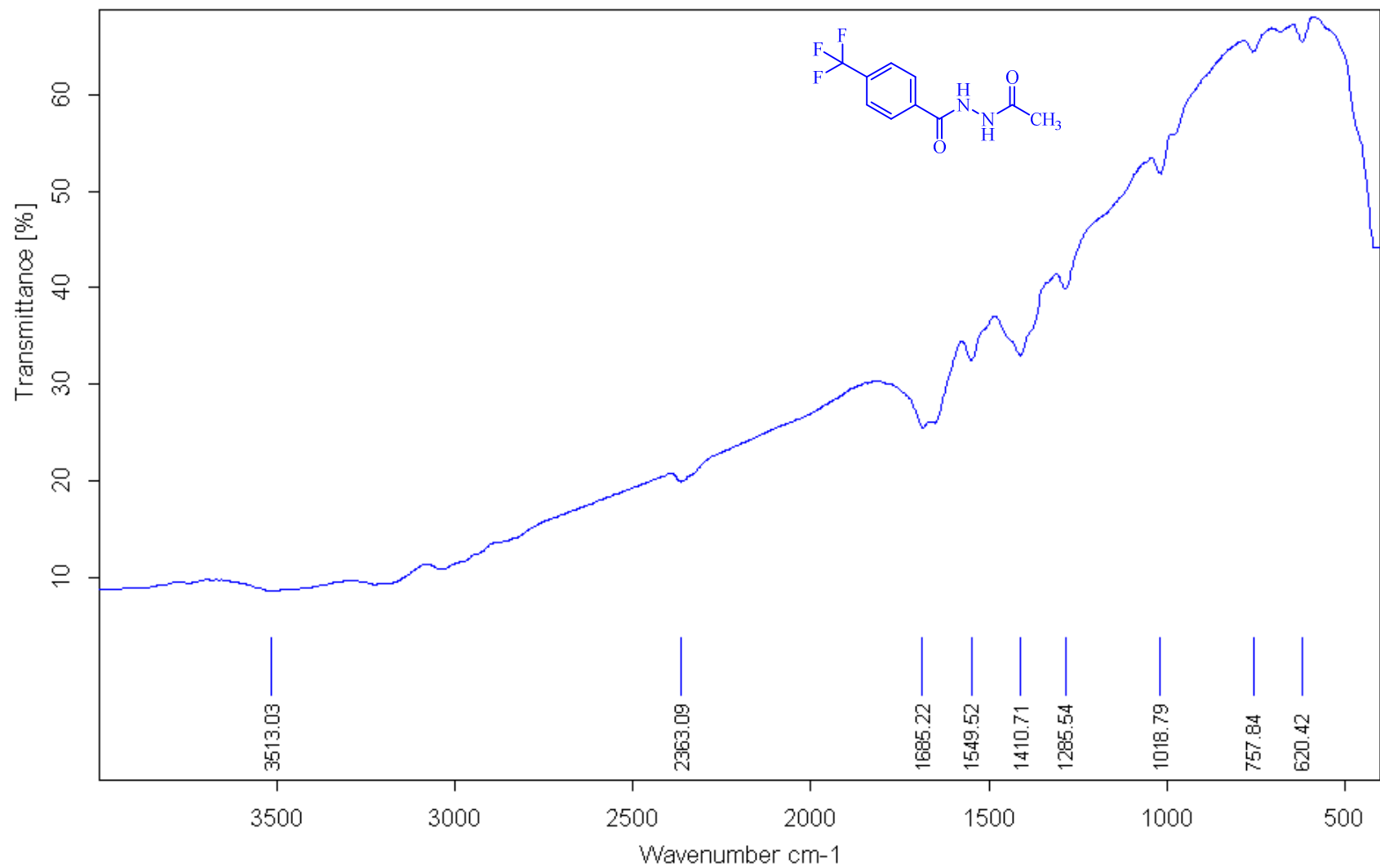


Fig. 33 FT-IR of *N'*-acetyl-4-(trifluoromethyl)benzohydrazide (**2k**)

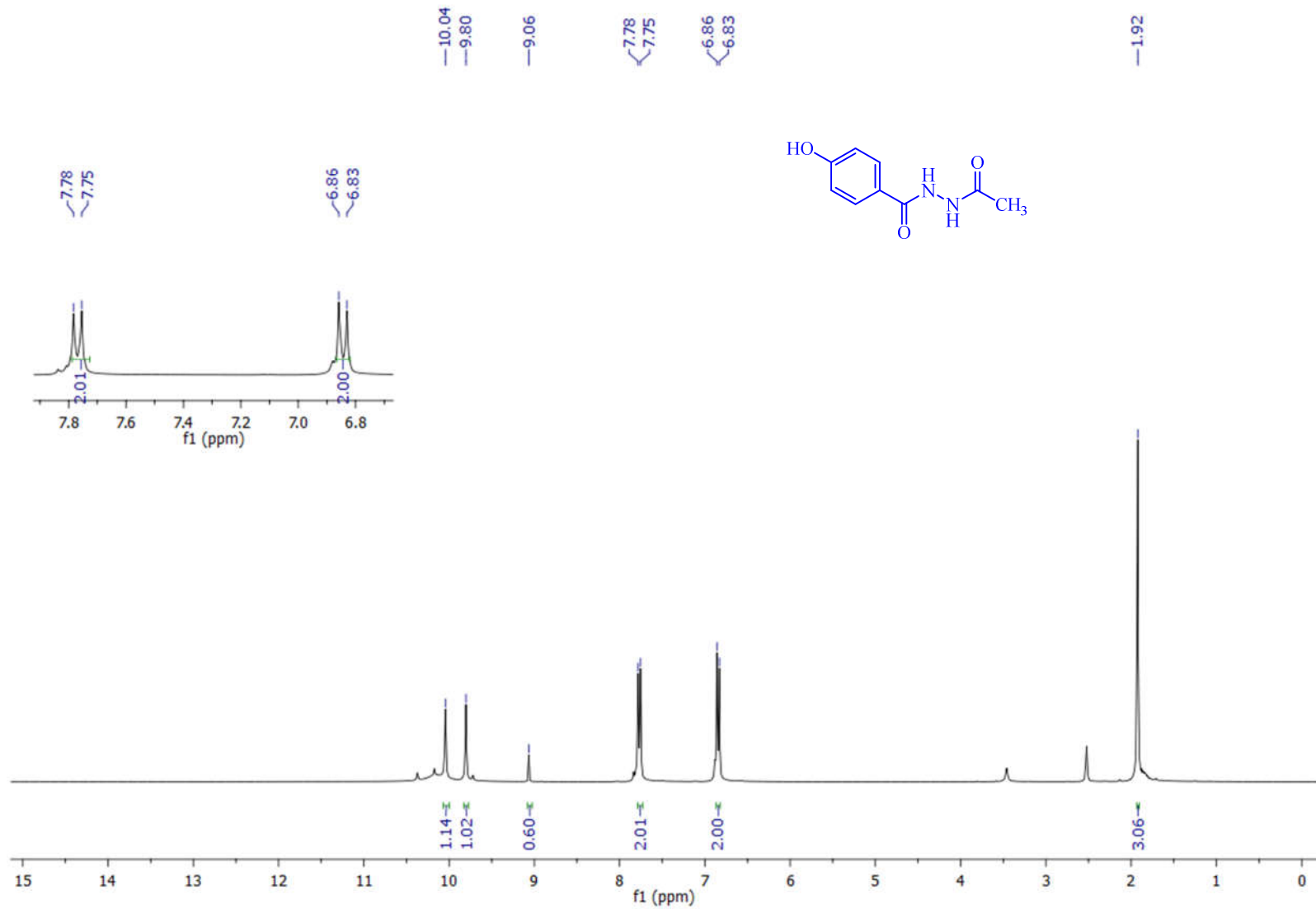


Fig. 34 ^1H NMR of *N'*-acetyl-4-hydroxybenzohydrazide (**21**)

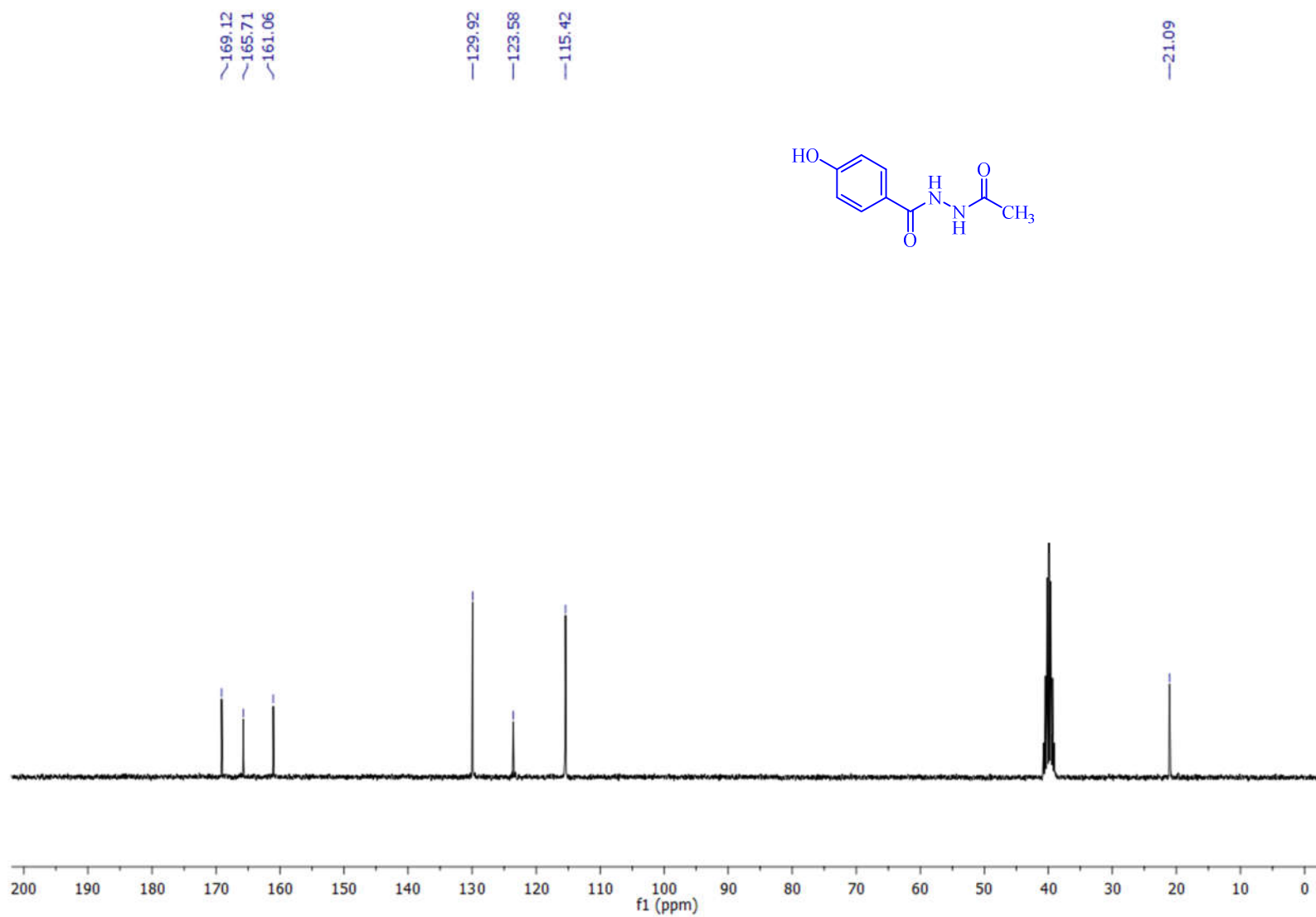


Fig. 35 ^{13}C NMR of *N'*-acetyl-4-hydroxybenzohydrazide (**2I**)

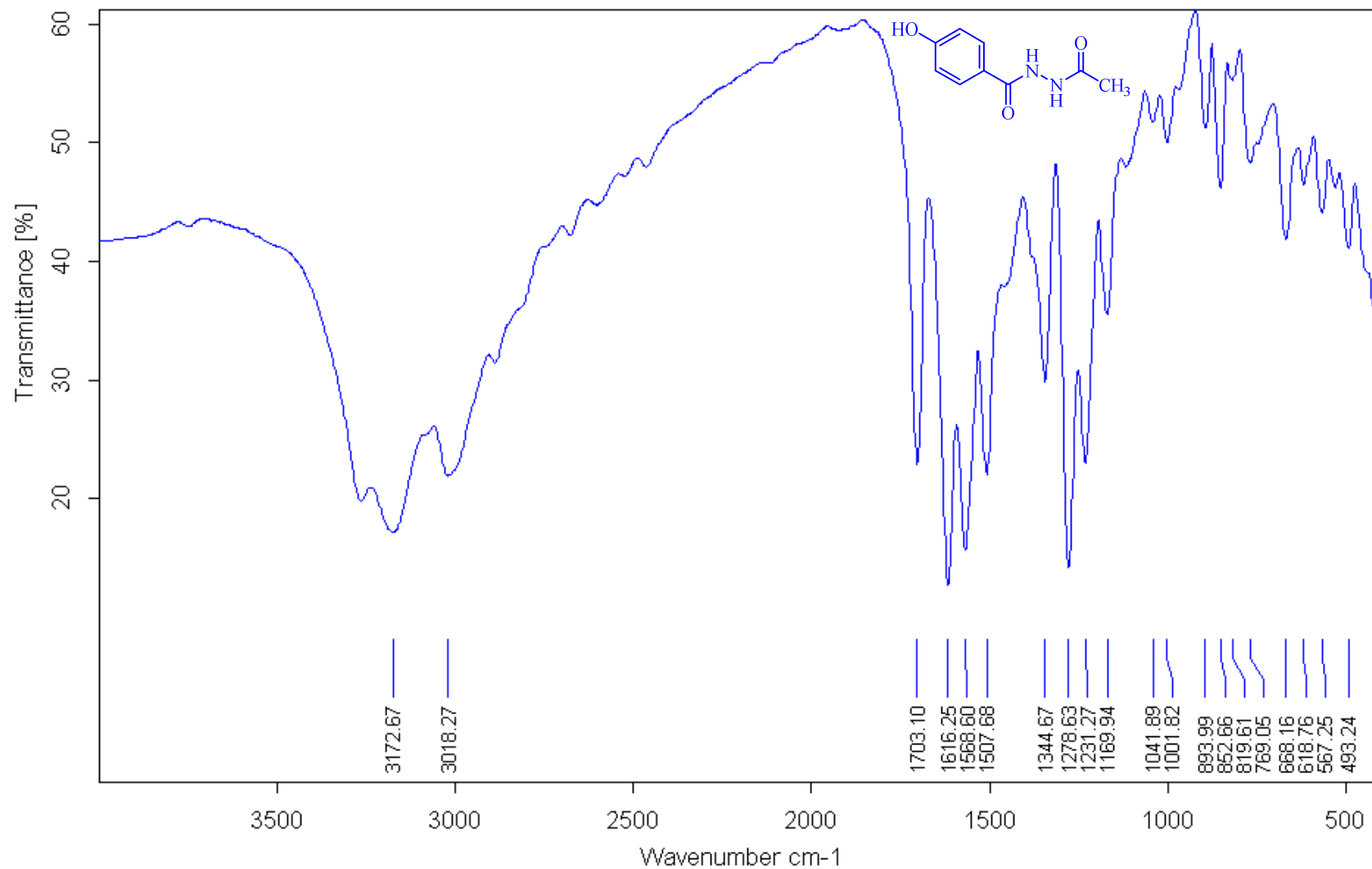


Fig. 36 FT-IR of *N'*-acetyl-4-hydroxybenzohydrazide (**21**)

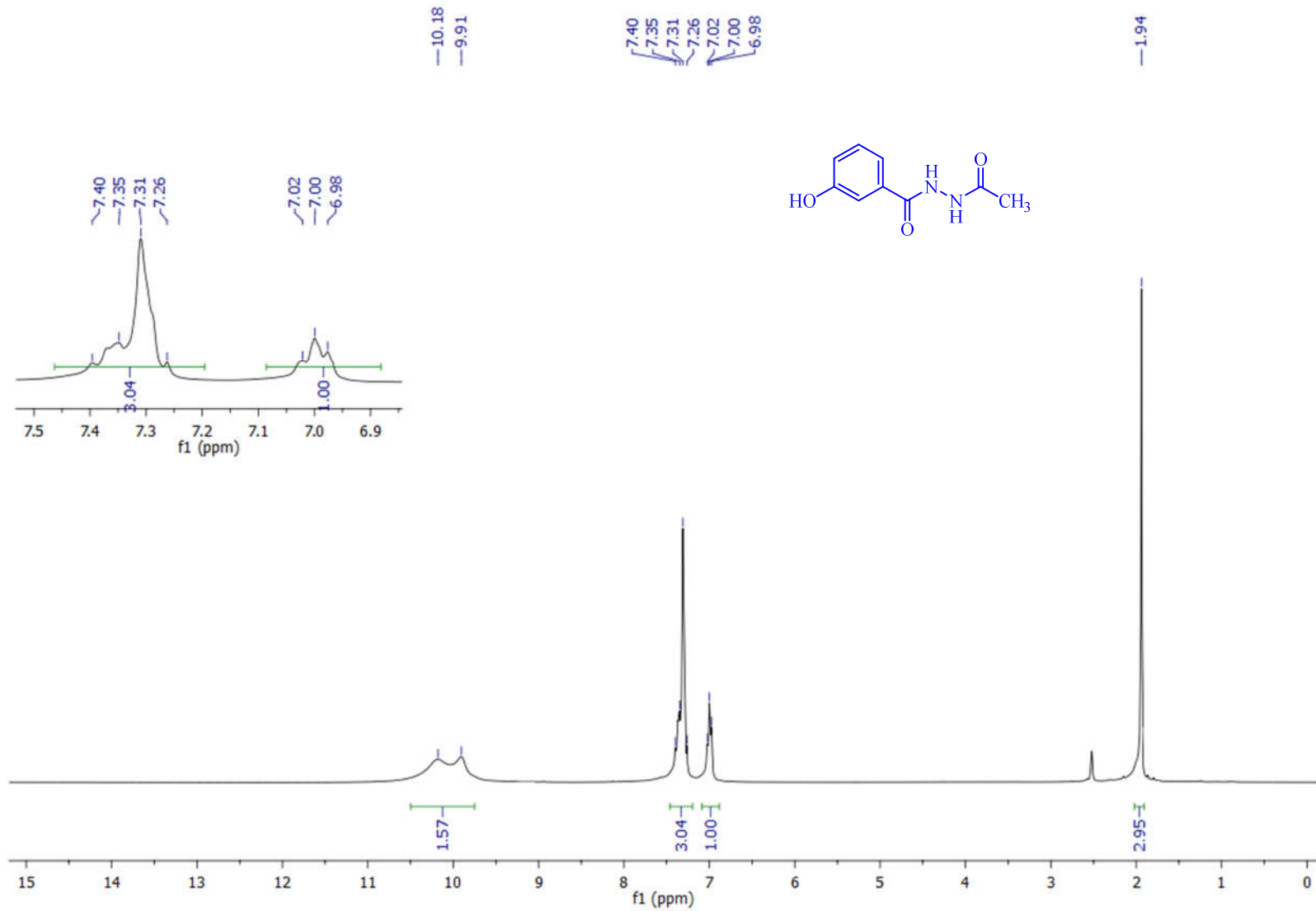


Fig. 37 ¹H NMR of *N'*-acetyl-3-hydroxybenzohydrazide (**2m**)

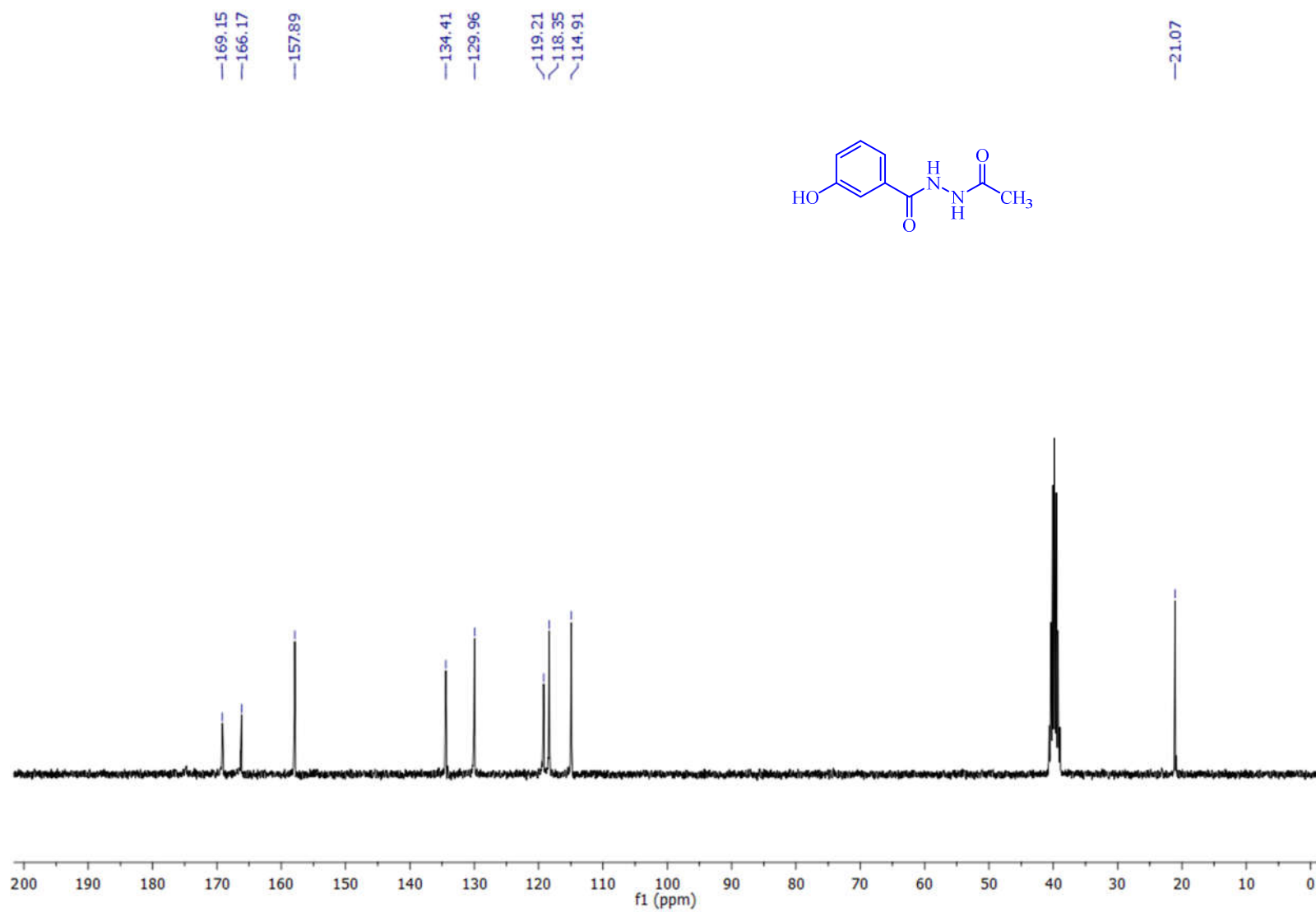


Fig. 38 ^{13}C NMR of *N'*-acetyl-3-hydroxybenzohydrazide (**2m**)

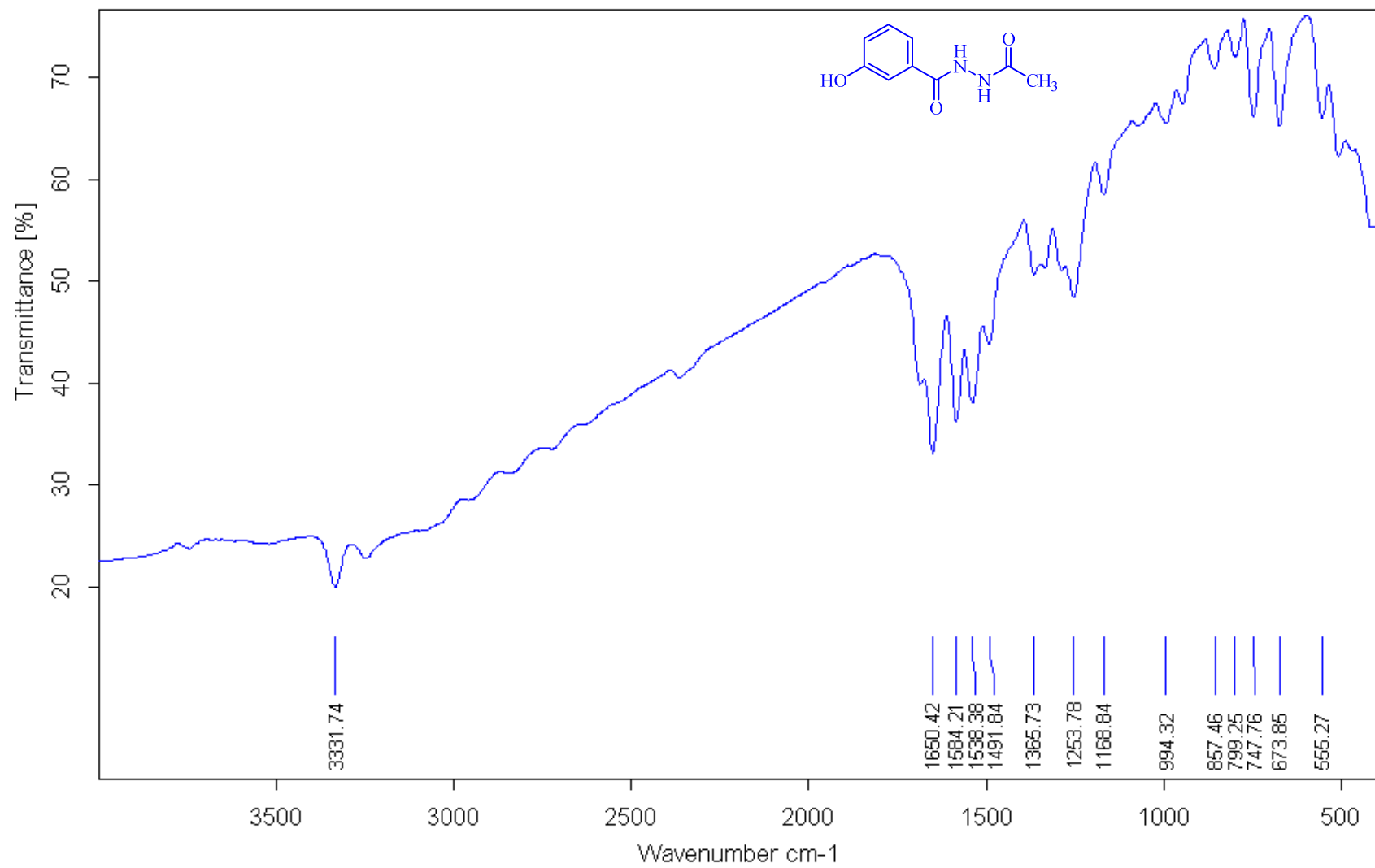


Fig. 39 FT-IR of *N'*-acetyl-3-hydroxybenzohydrazide (**2m**)

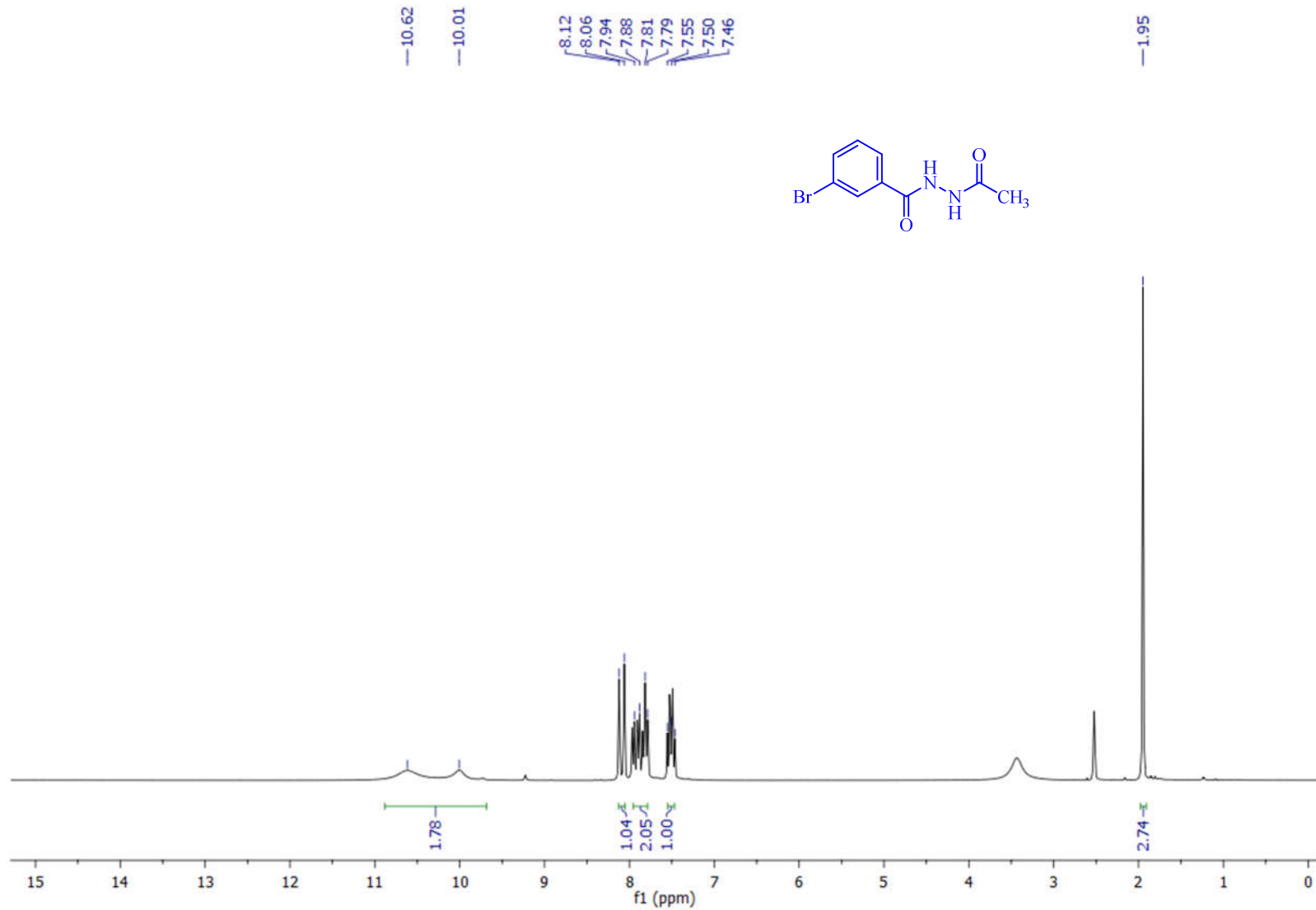


Fig. 40 ¹H NMR of *N'*-acetyl-3-bromobenzohydrazide (**2n**)

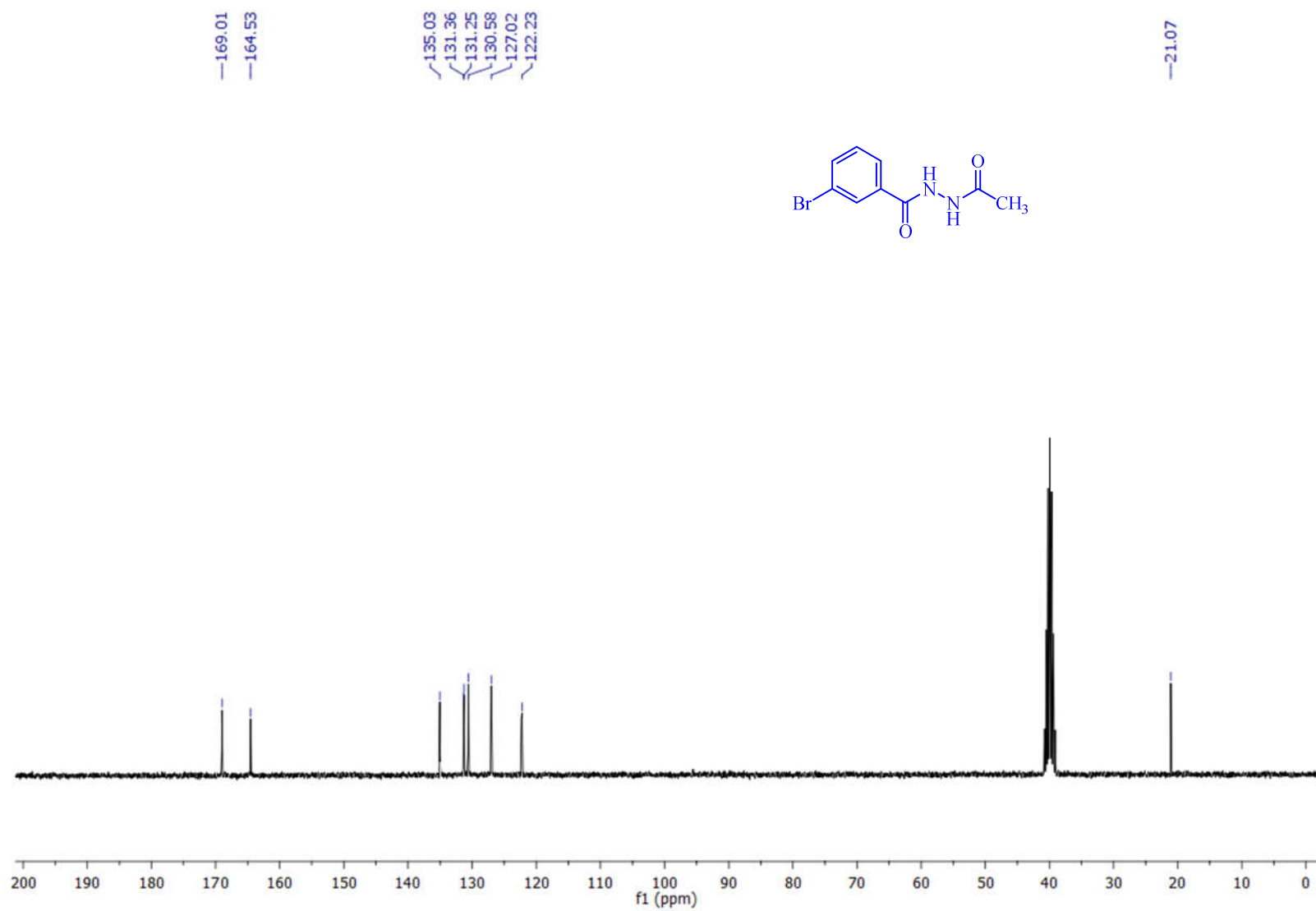


Fig. 41 ¹³C NMR of *N'*-acetyl-3-bromobenzohydrazide (2n)

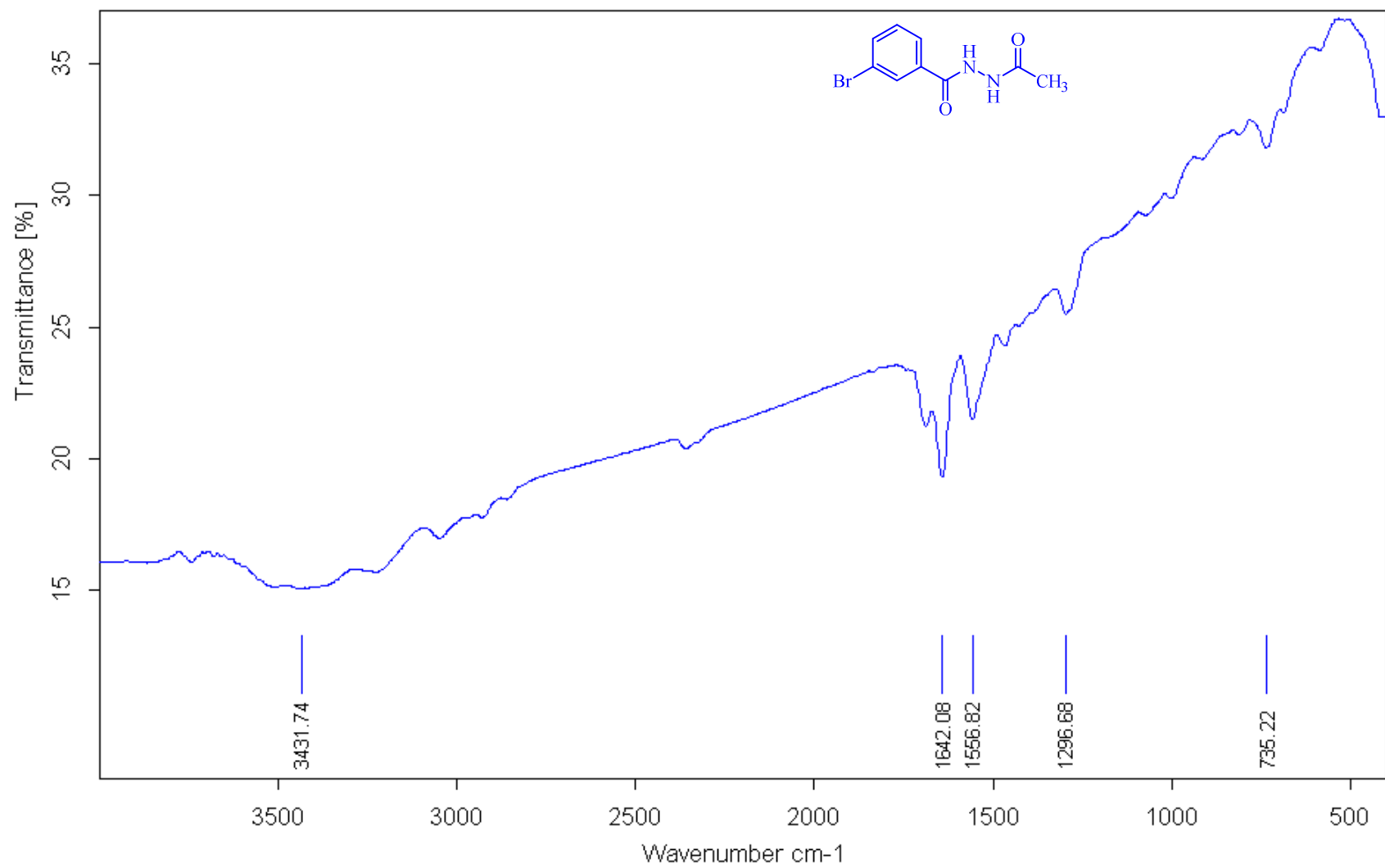


Fig. 42 FT-IR of *N'*-acetyl-3-bromobenzohydrazide (**2n**)

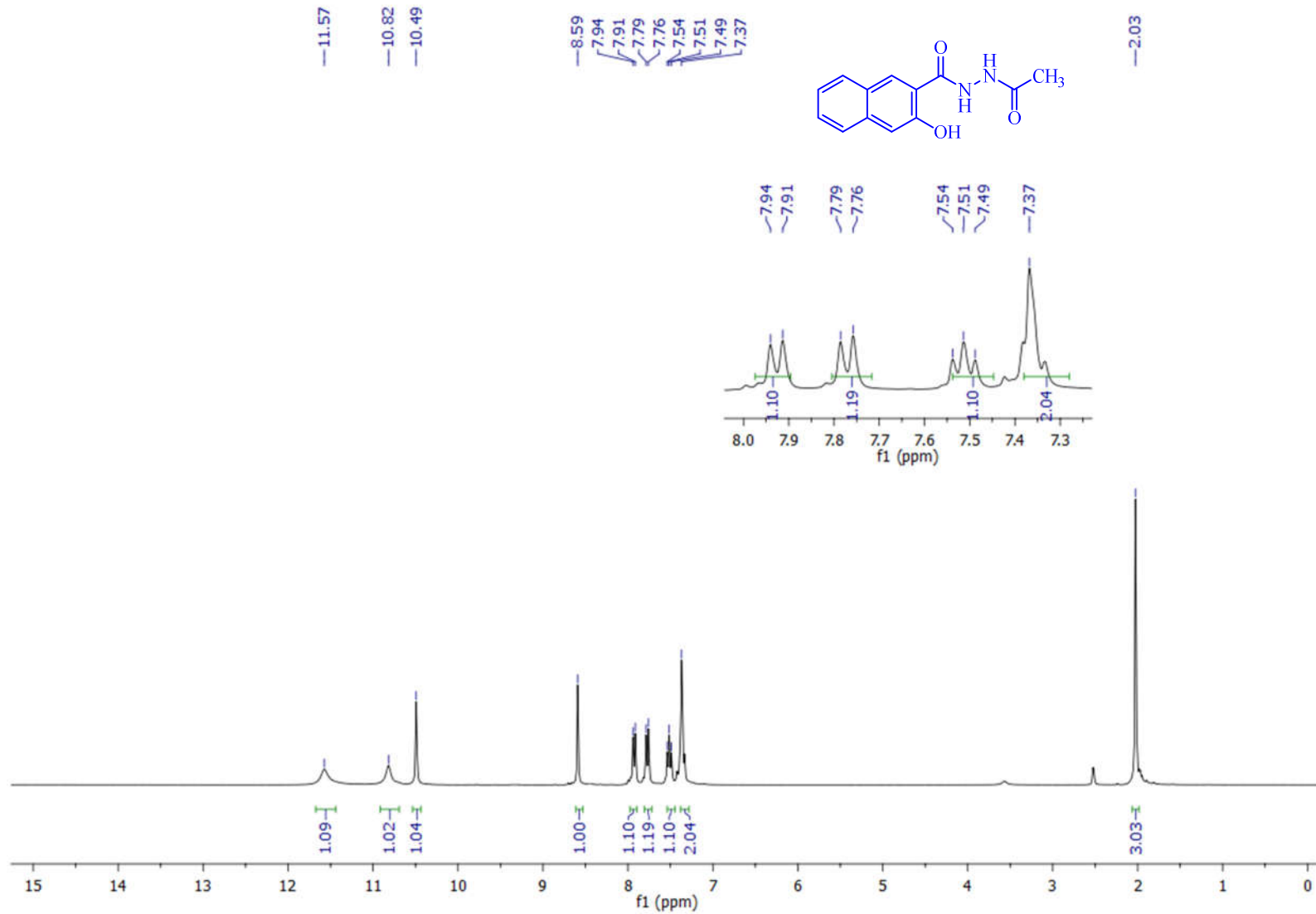


Fig. 43 ¹H NMR of *N'*-acetyl-3-hydroxy-2-naphthohydrazide (**2o**)

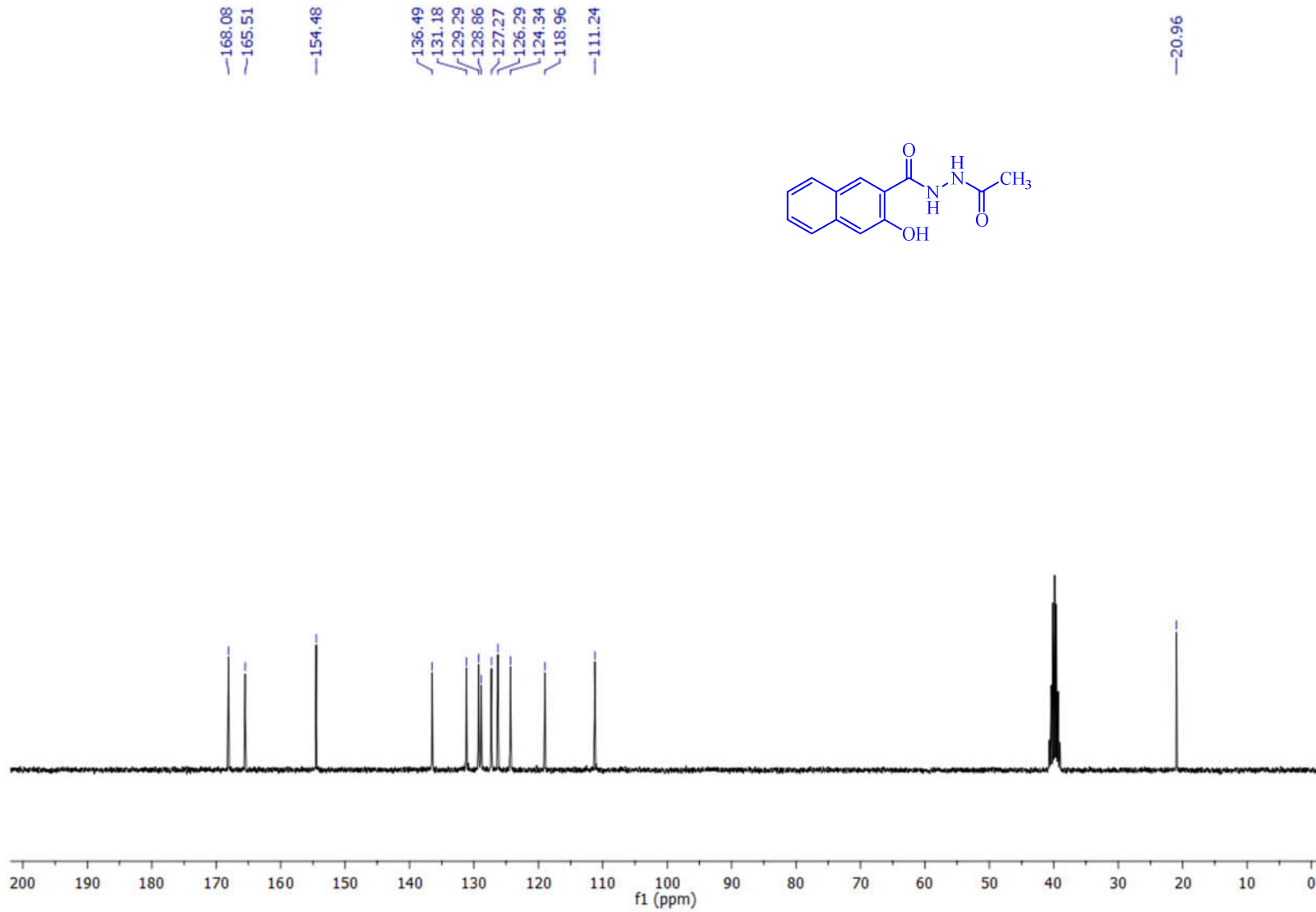


Fig. 44 ¹³C NMR of *N'*-acetyl-3-hydroxy-2-naphthohydrazide (**2o**)

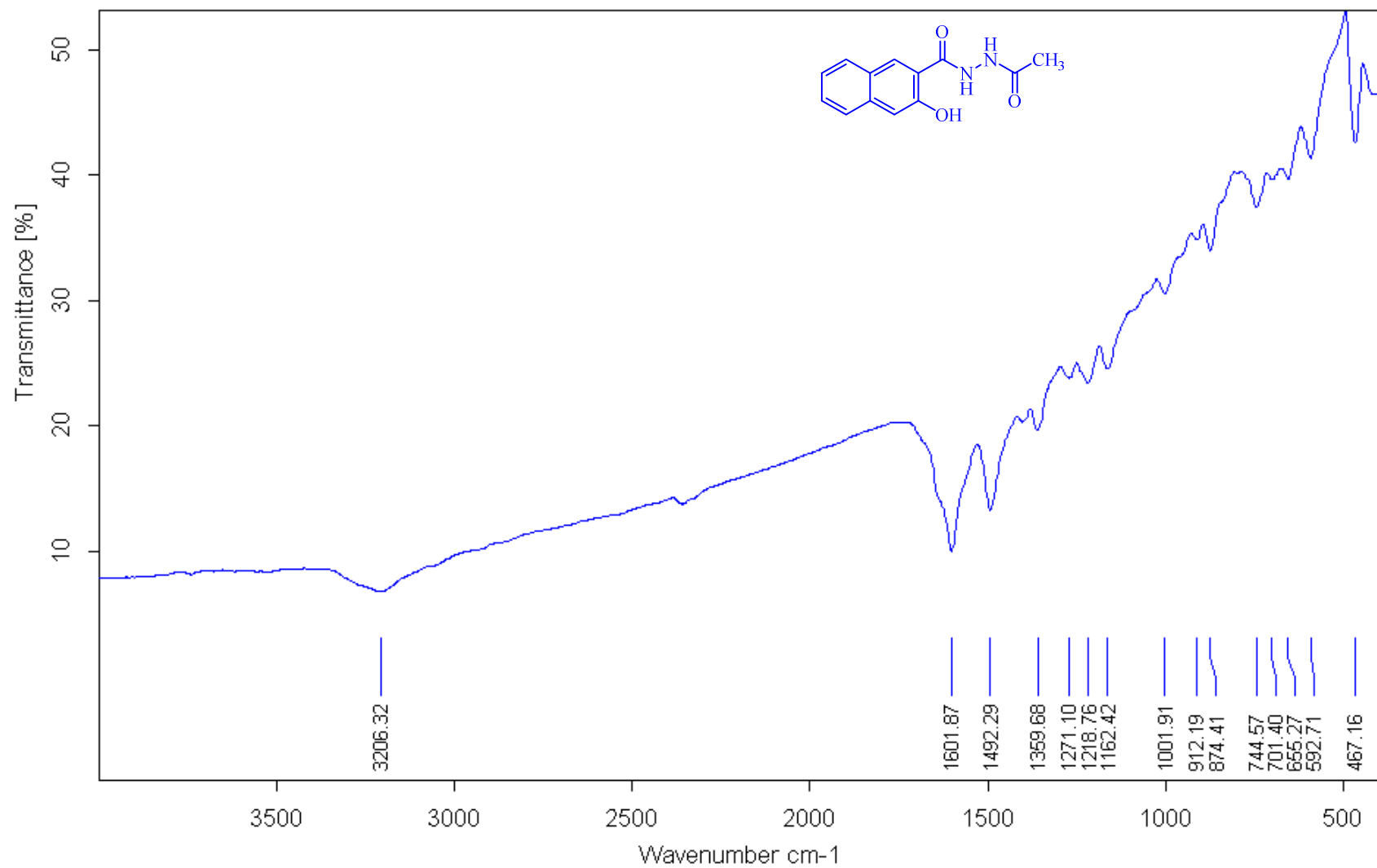


Fig. 45 FT-IR of *N'*-acetyl-3-hydroxy-2-naphthohydrazide (**2o**)

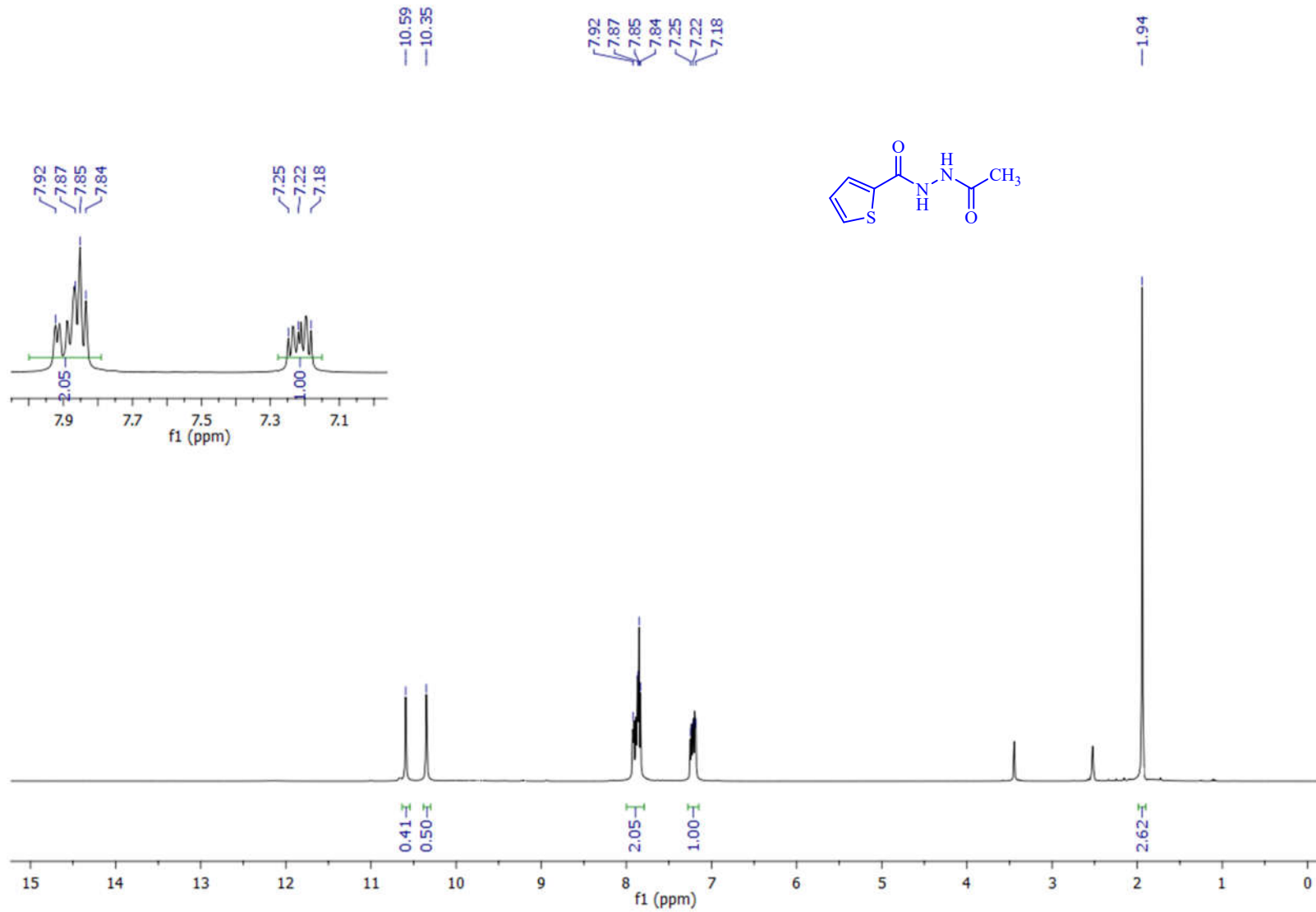


Fig. 46 ¹H NMR of *N'*-acetylthiophene-2-carbohydrazide (**2p**)

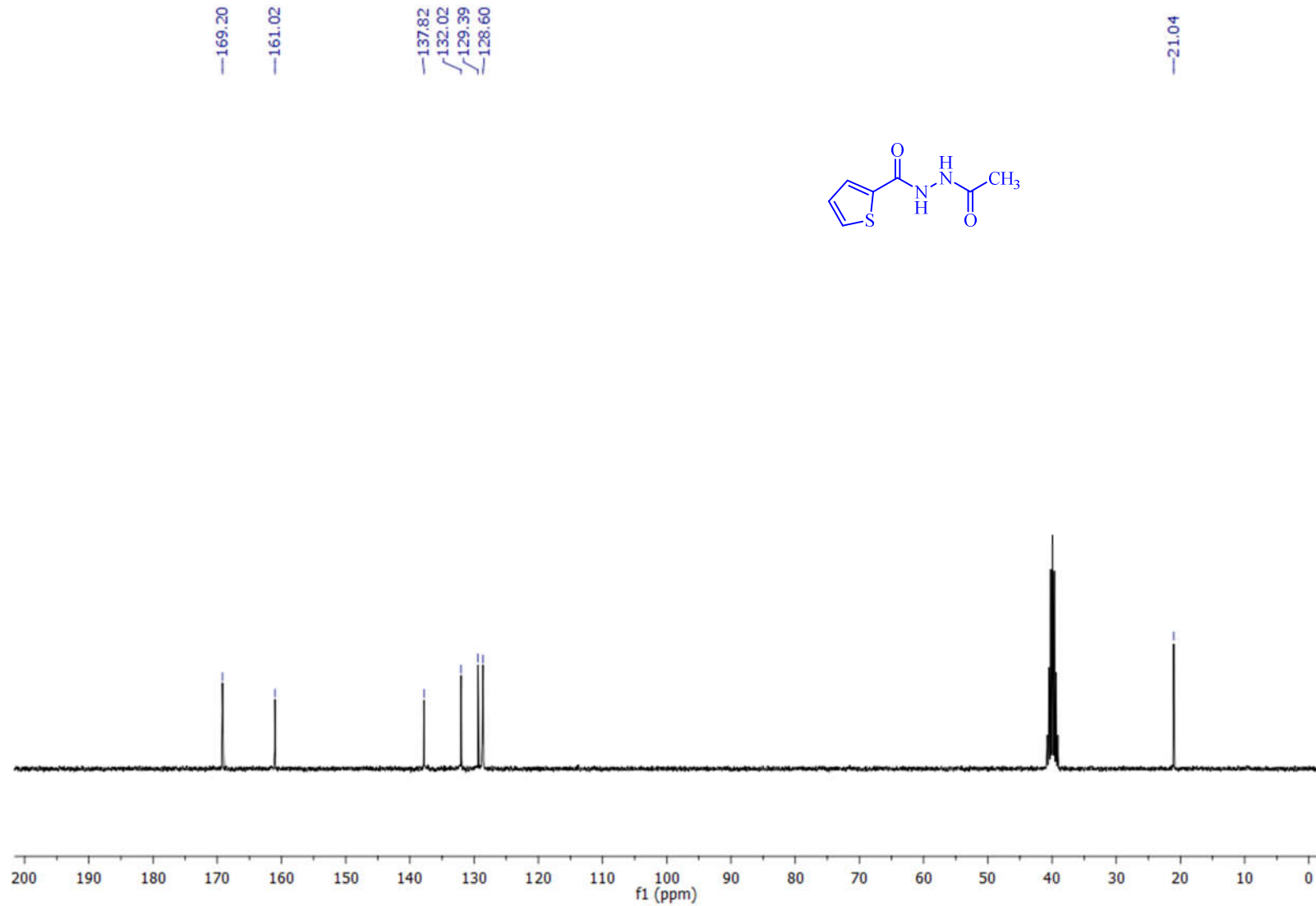


Fig. 47 ¹³C NMR of *N'*-acetylthiophene-2-carbohydrazide (2p)

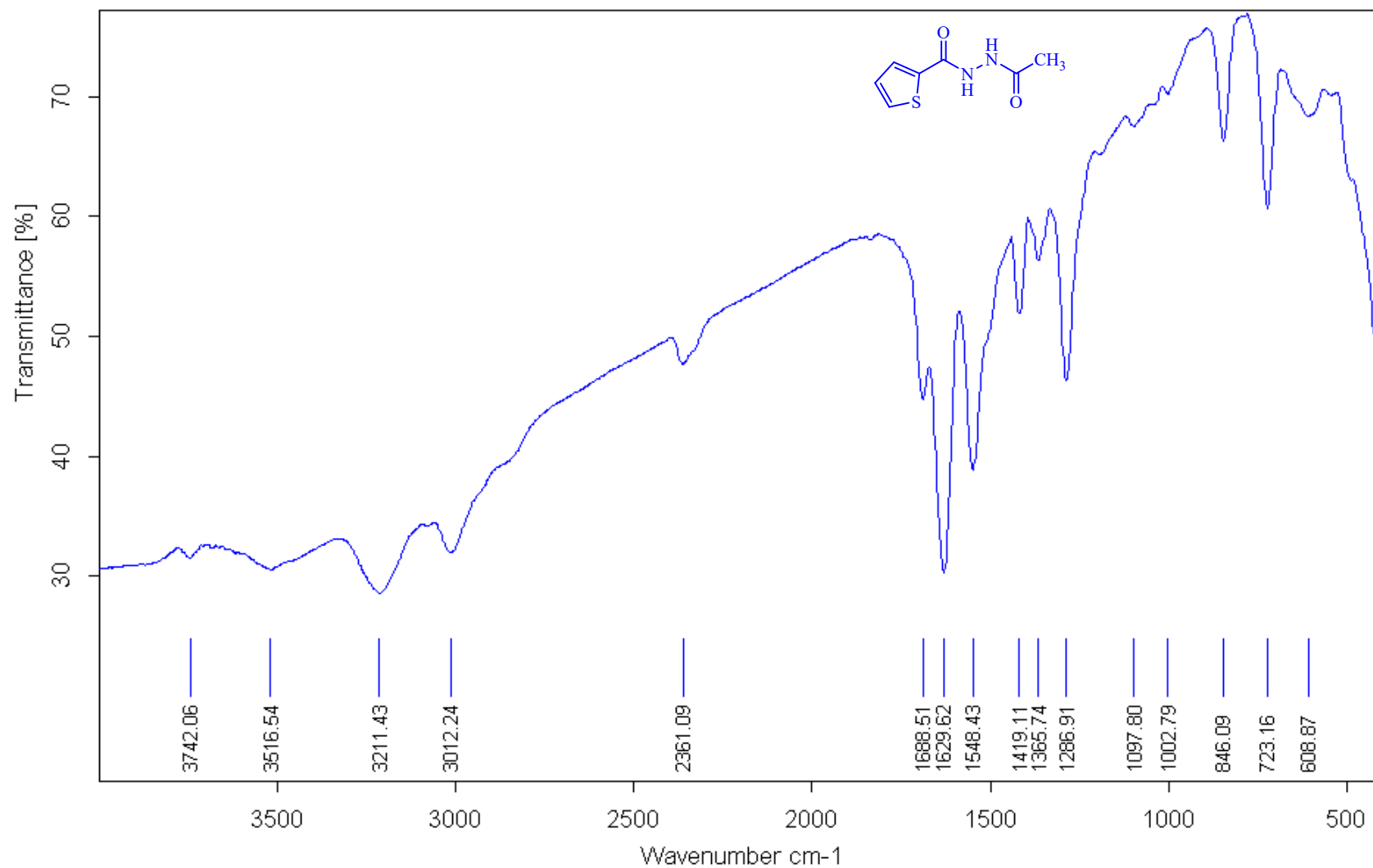


Fig. 48 FT-IR of *N'*-acetylthiophene-2-carbohydrazide (**2p**)

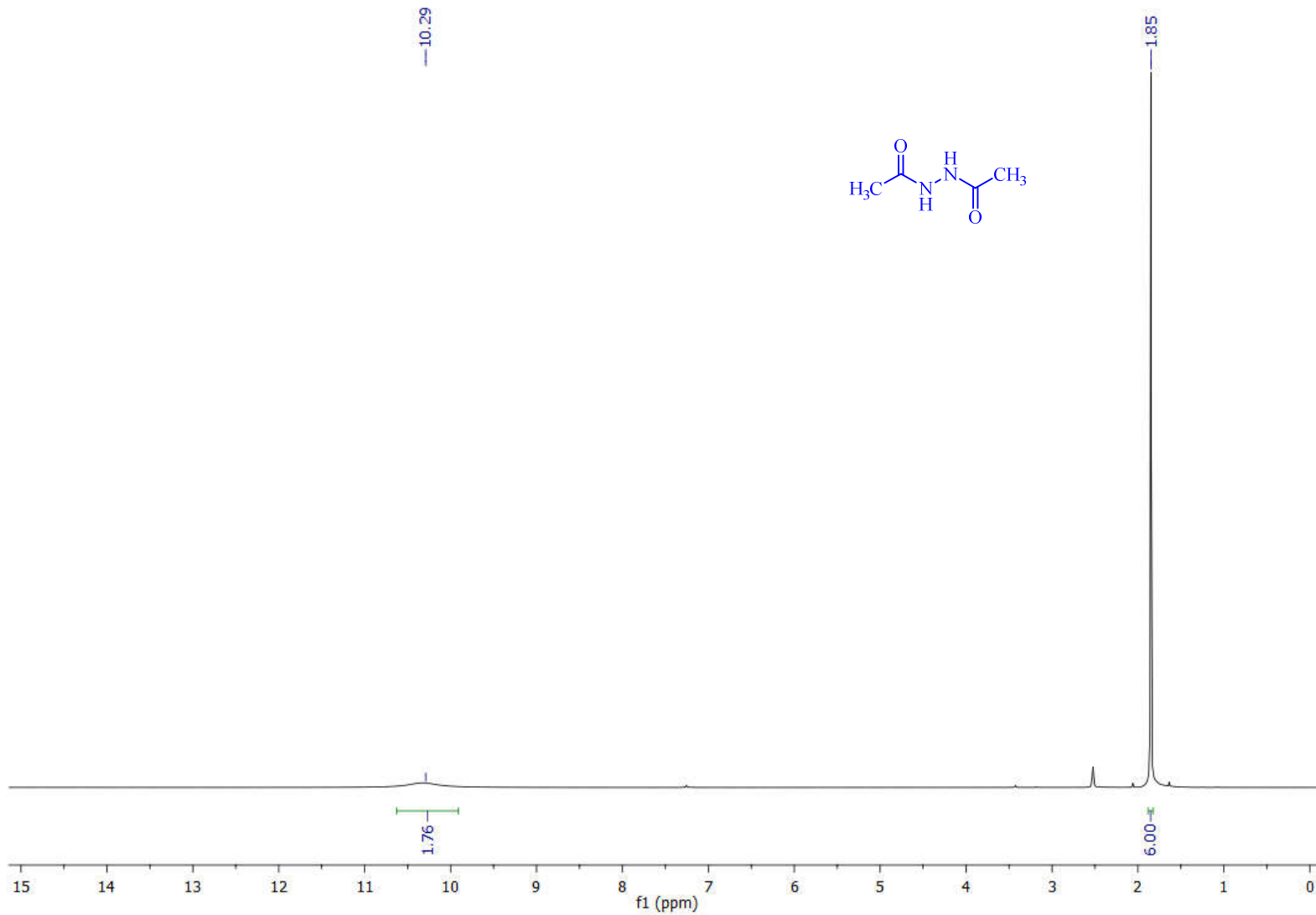


Fig. 49 ^1H NMR of *N'*-acetylacetohydrazide (**2q**)

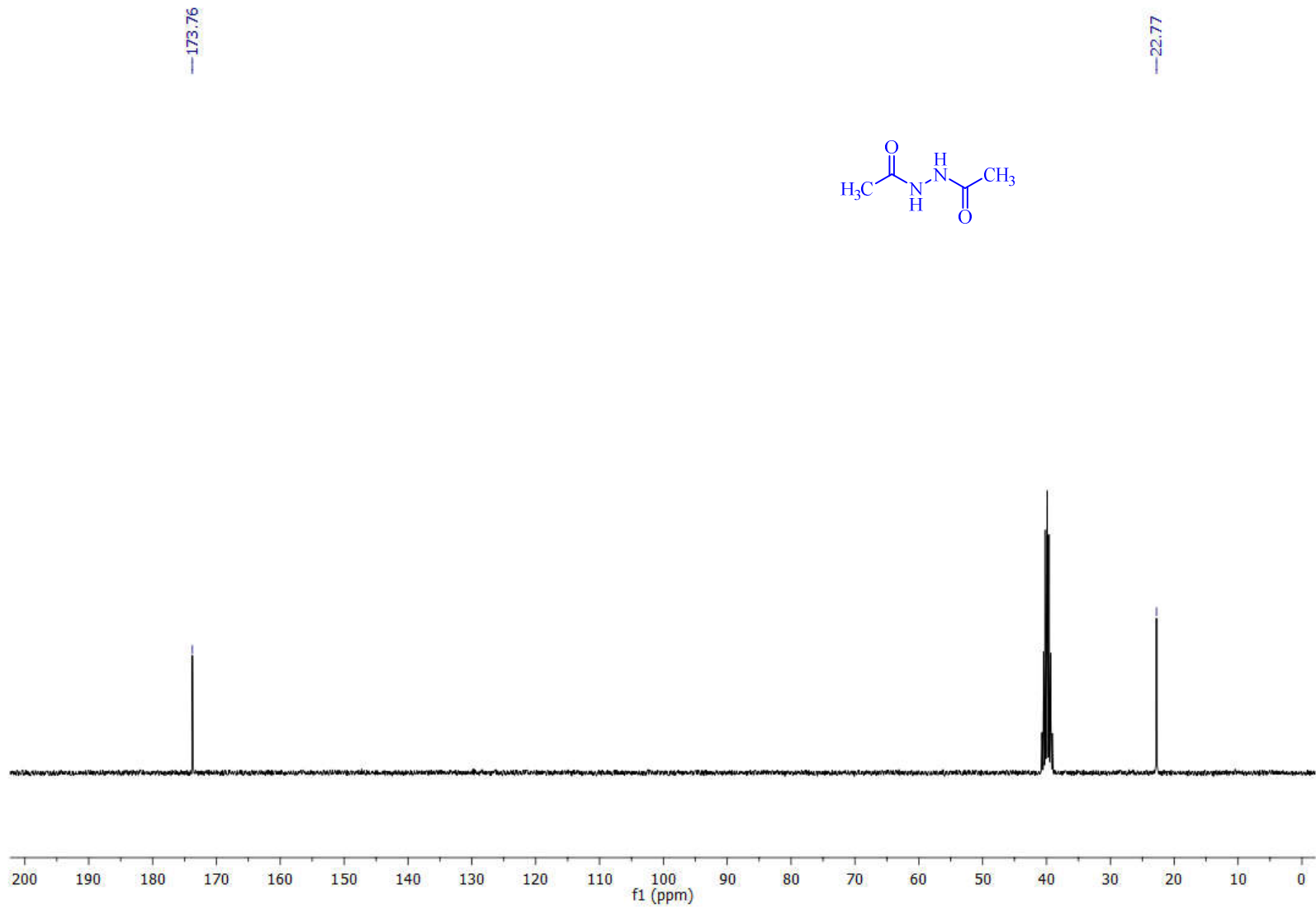


Fig. 50 ^{13}C NMR of *N'*-acetylacetohydrazide (2q)

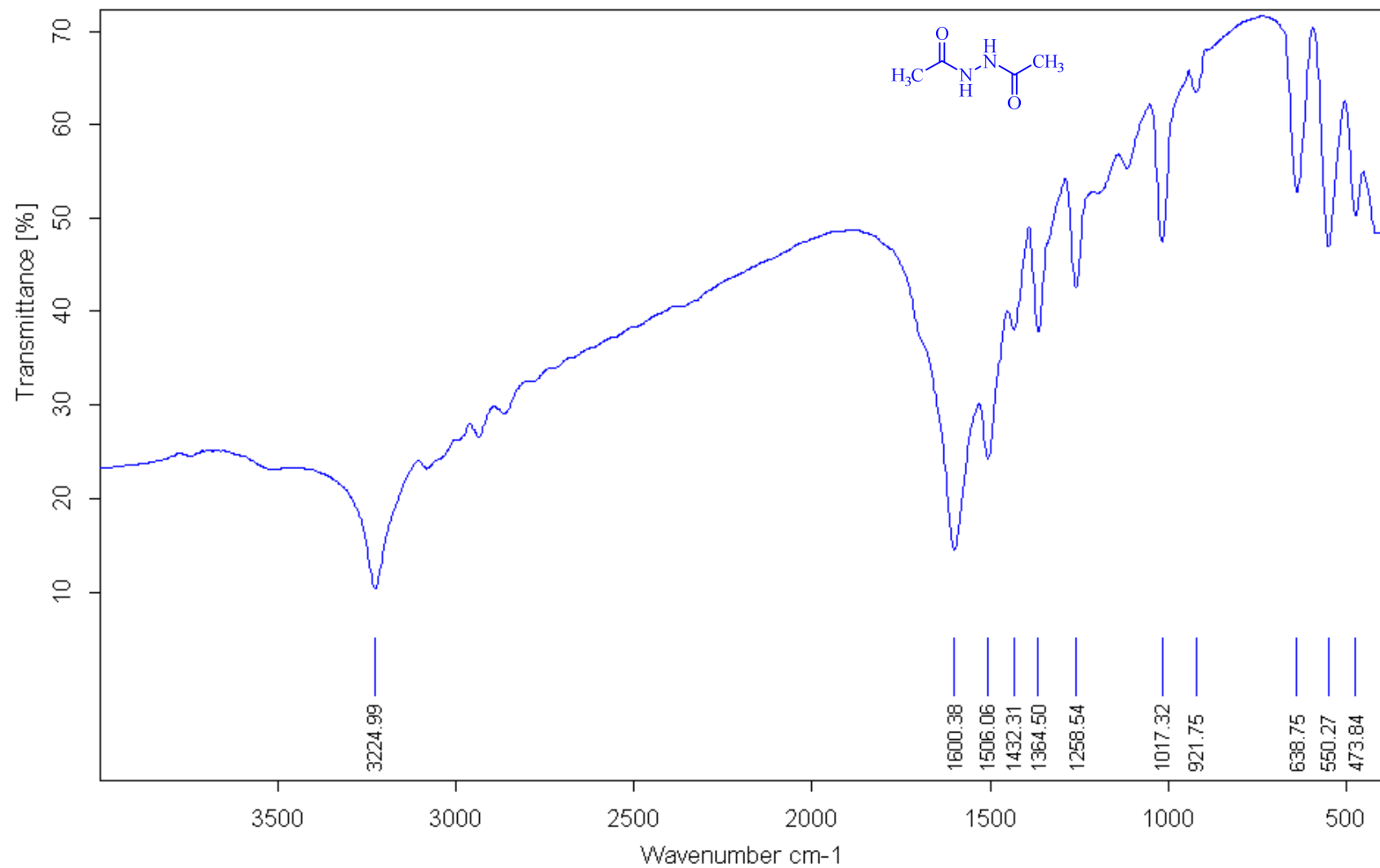


Fig. 51 FT-IR of *N'*-acetylacetohydrazide (**2q**)