

Supplementary Information (NMR Charts)

Hydration of Nitriles to Amides by a Chitin-supported Ruthenium Catalyst

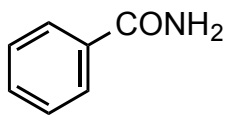
Aki Matsuoka^a, Takahiro Isogawa^a, Yuna Morioka^a, Benjamin R. Knappett^b, Andrew E. H. Wheatley^{*b},
Susumu Saito^{*ac}, and Hiroshi Naka^{*a}

^a Graduate School of Science and Research Center for Materials Science, Nagoya University, Chikusa,
Nagoya 464-8602, Japan

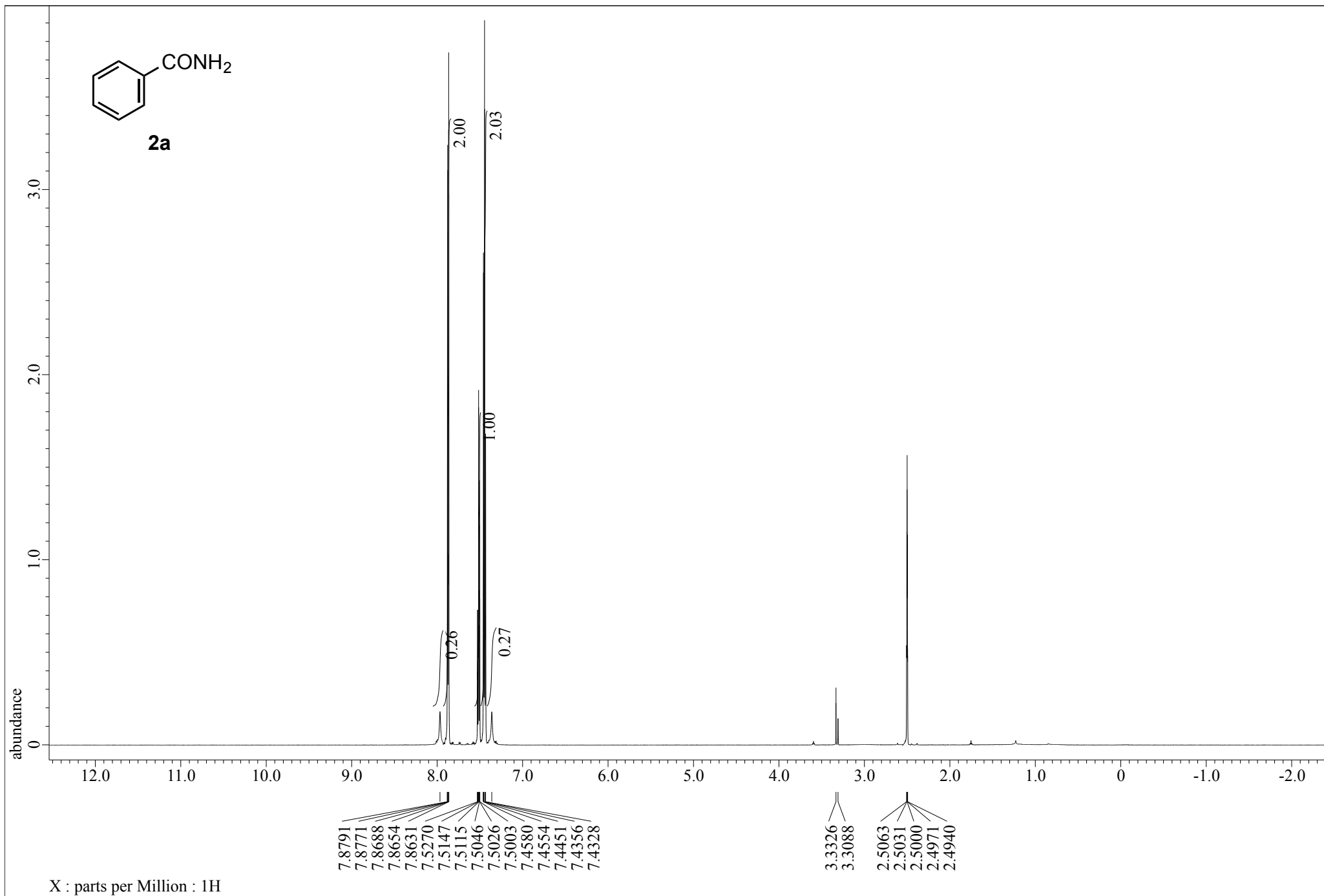
^b Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, UK

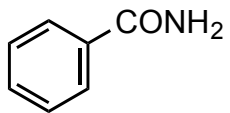
^c Institute for Advanced Research, Nagoya University, Chikusa, Nagoya 464-8601, Japan

h_naka@nagoya-u.jp

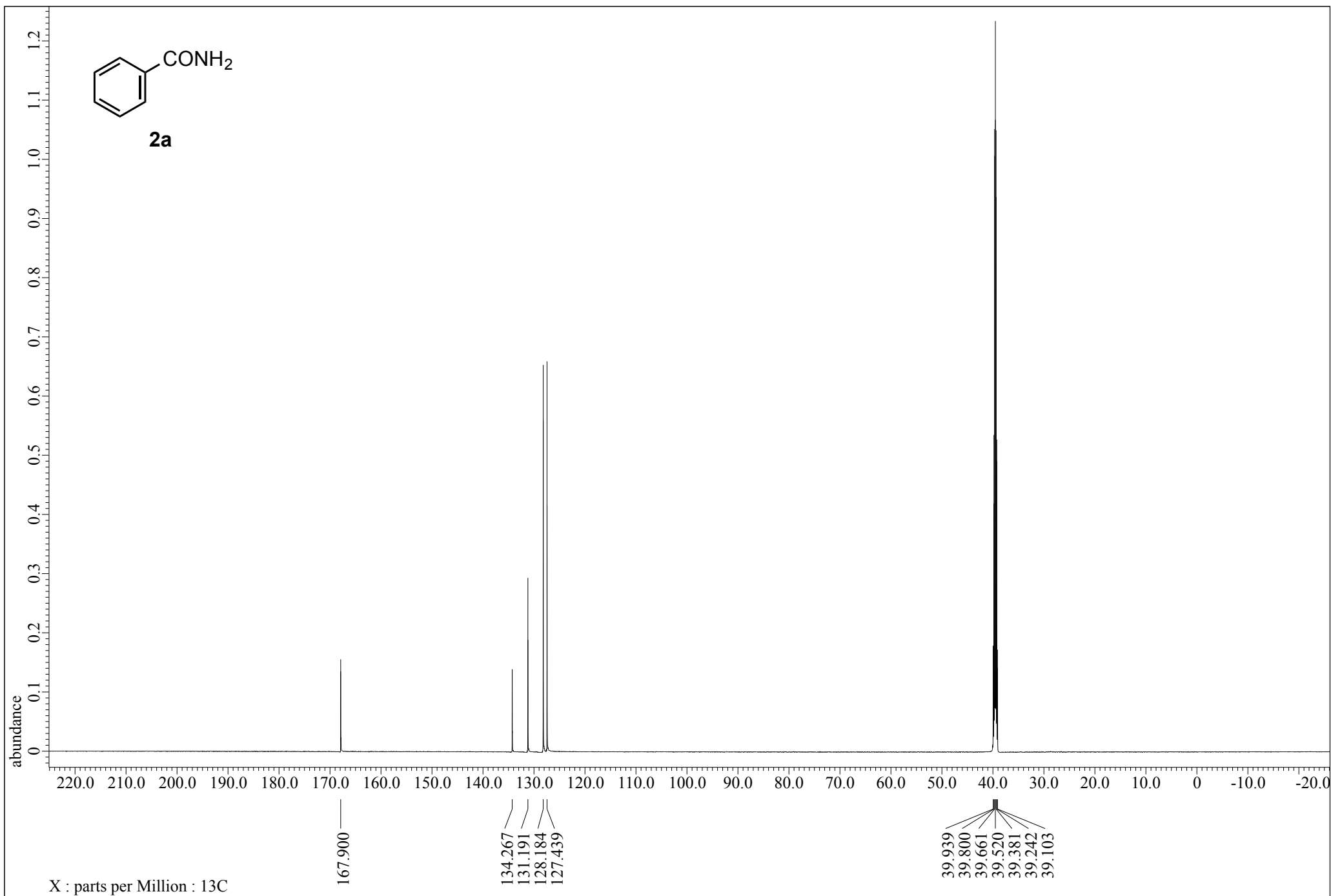


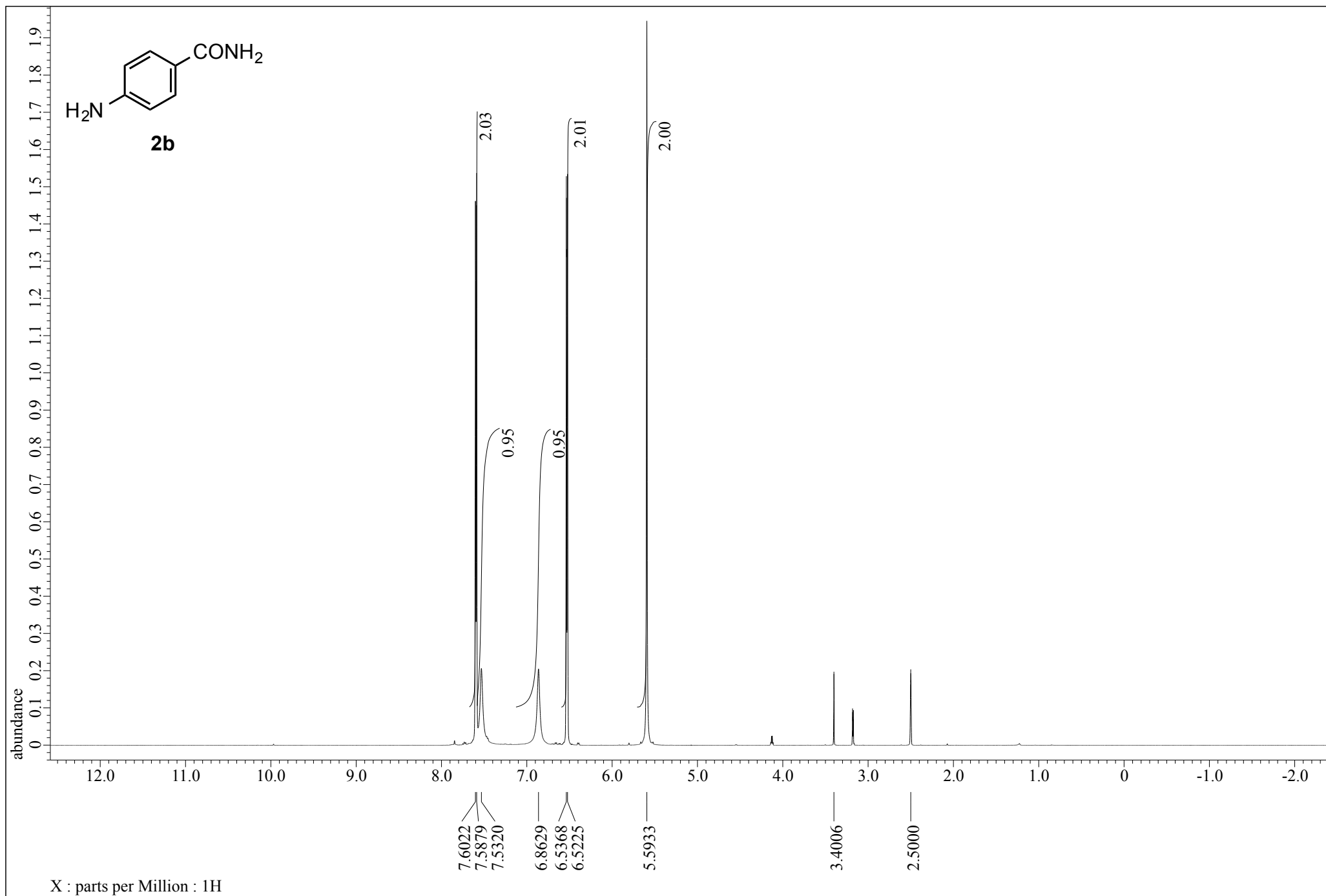
2a

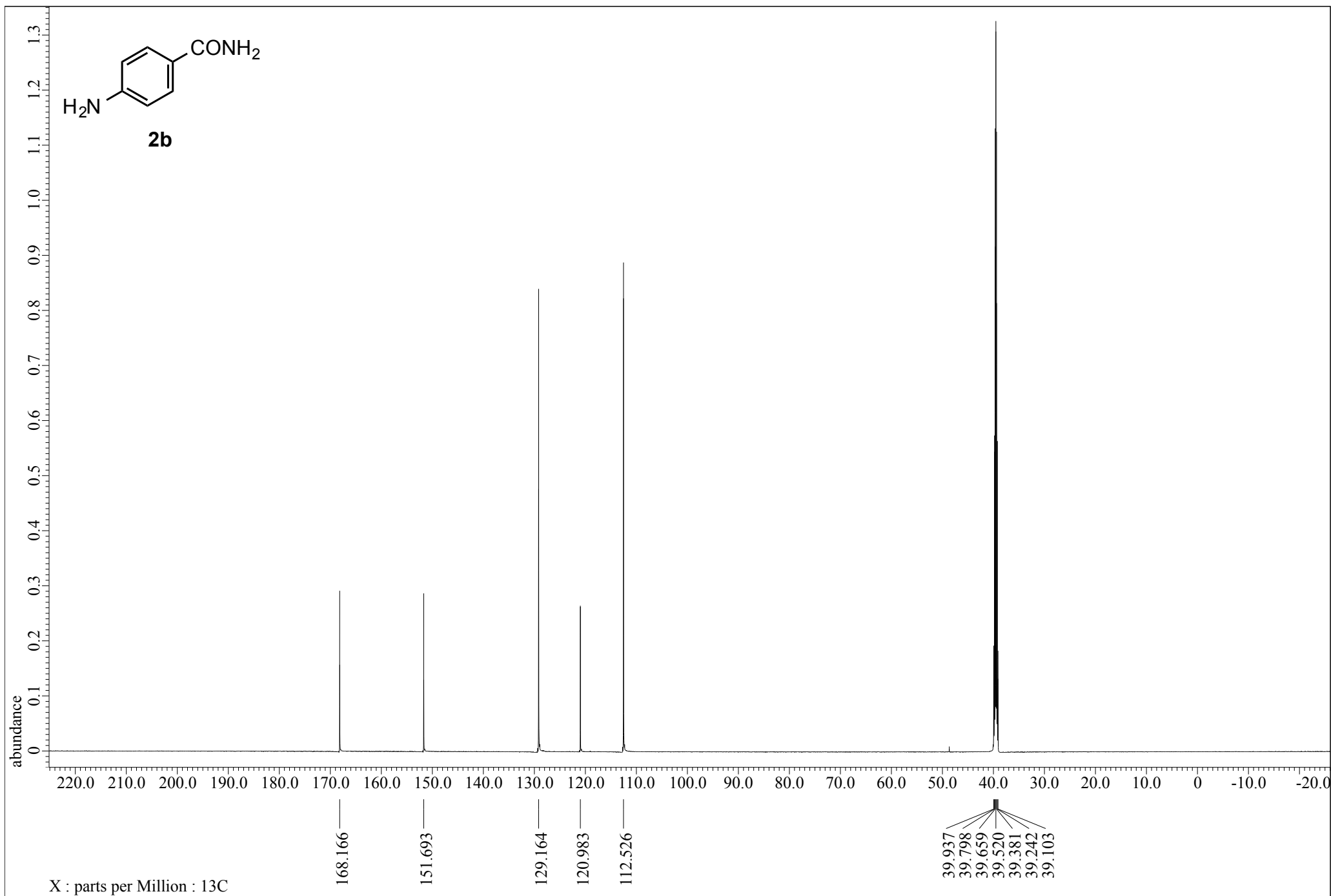


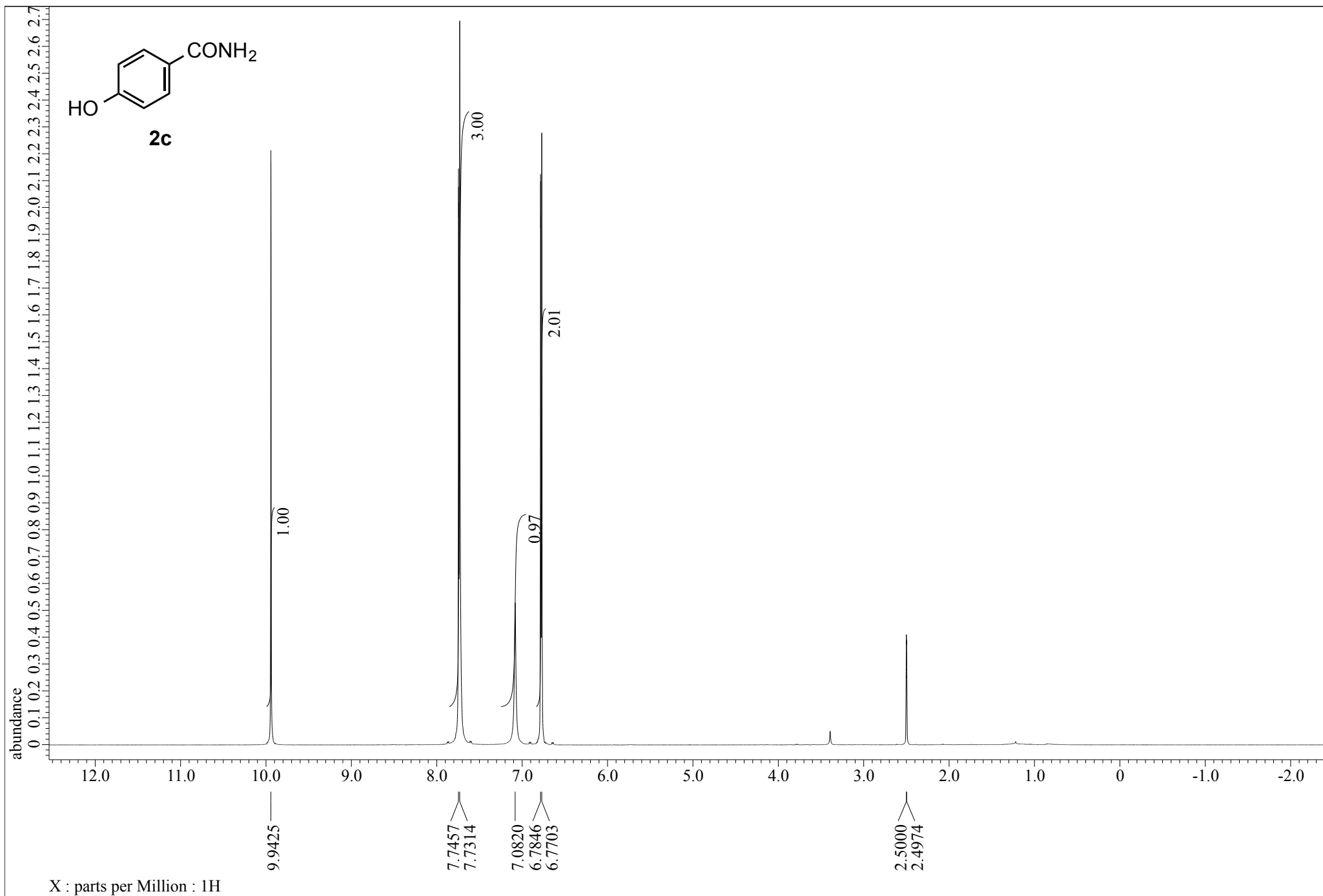


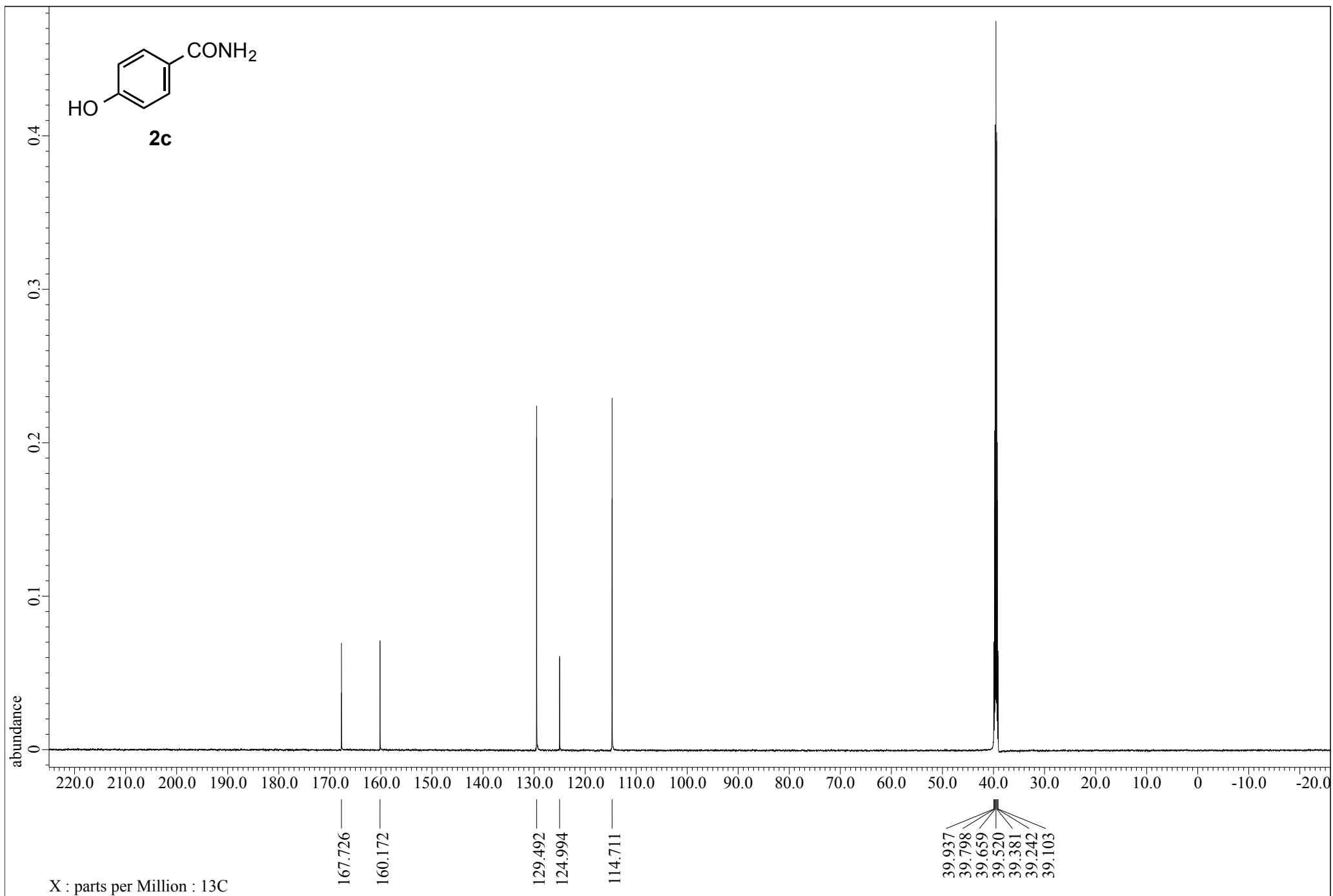
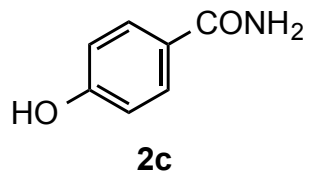
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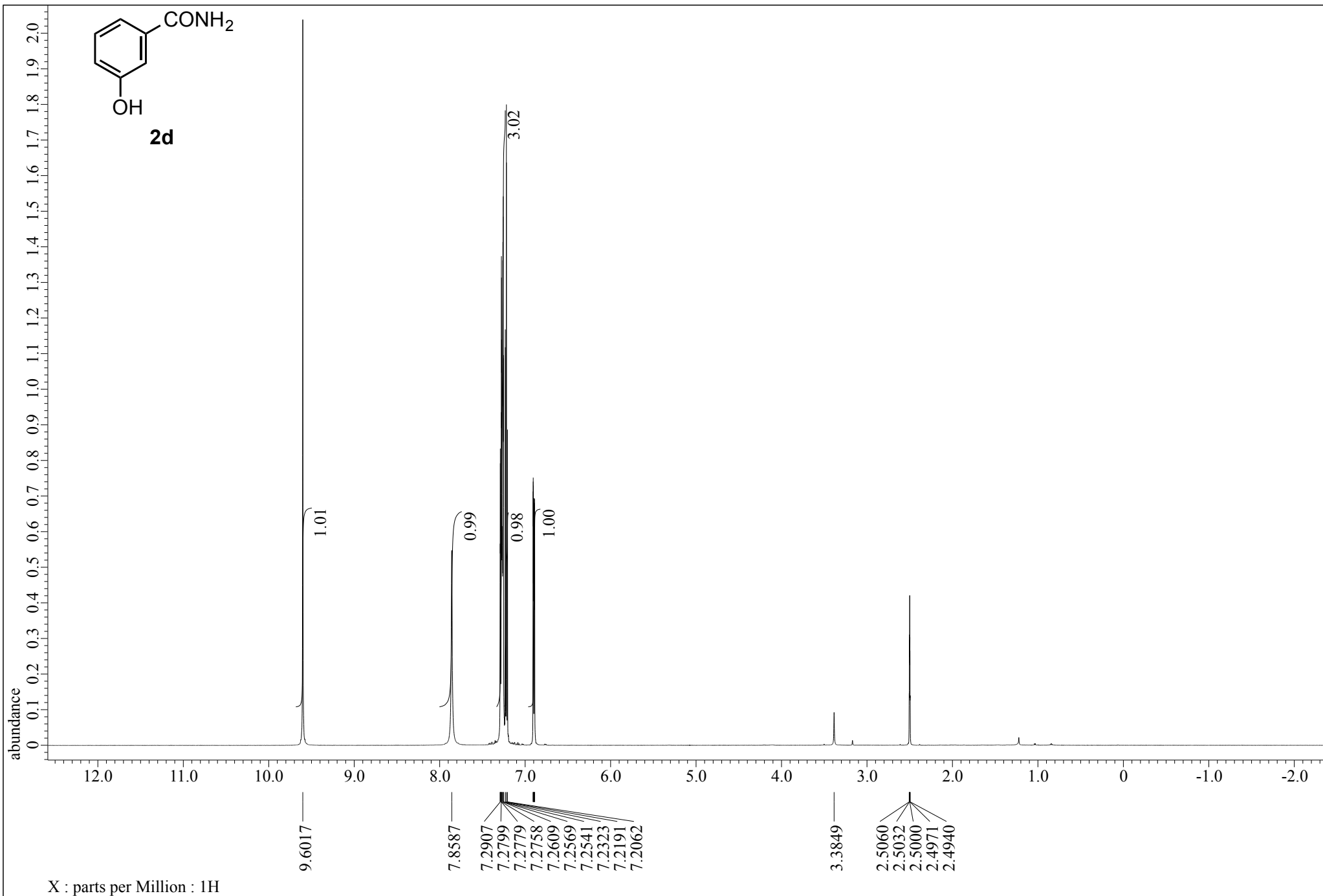
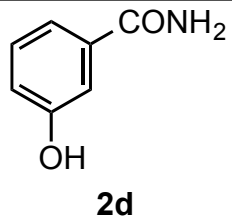


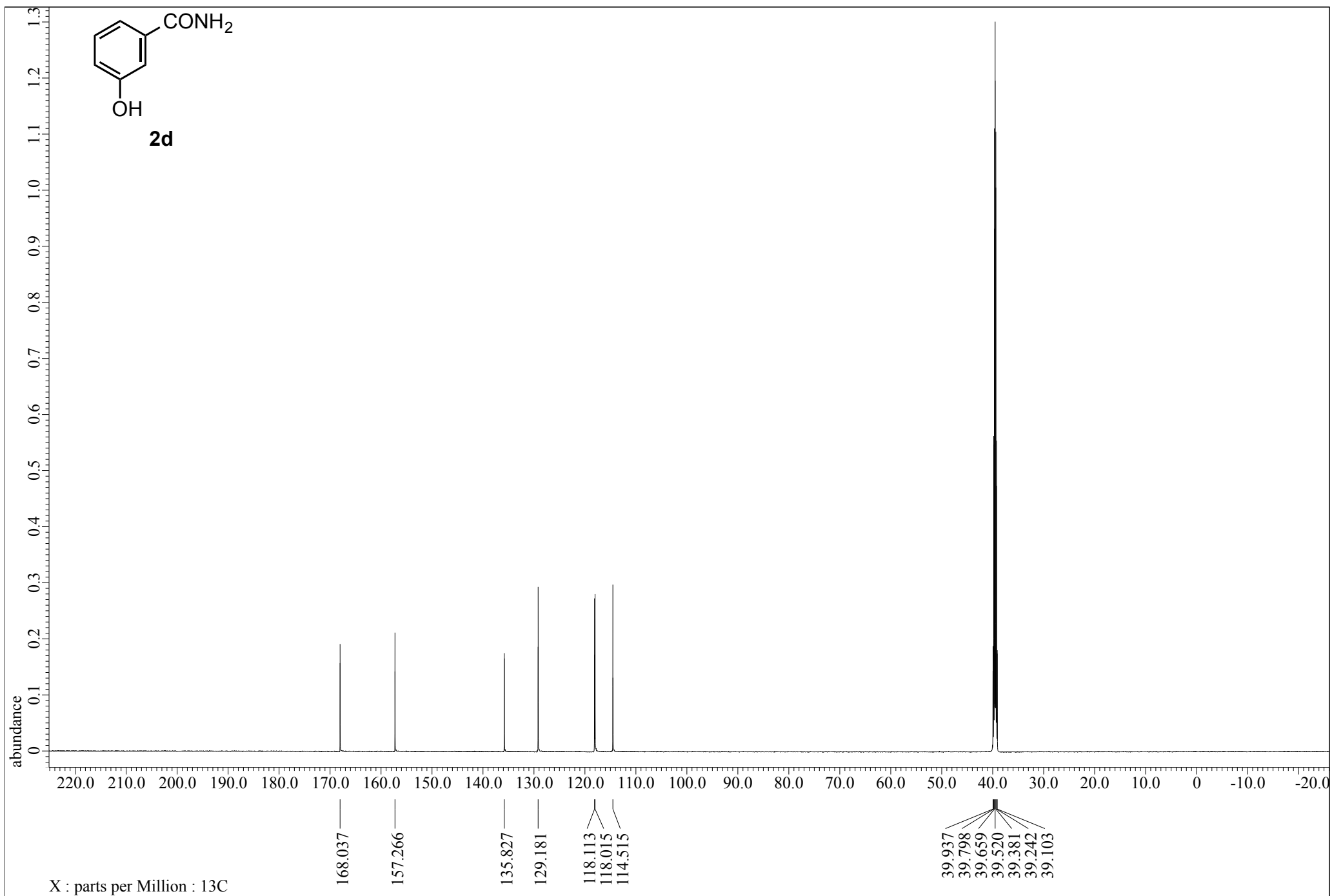
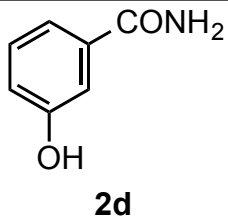


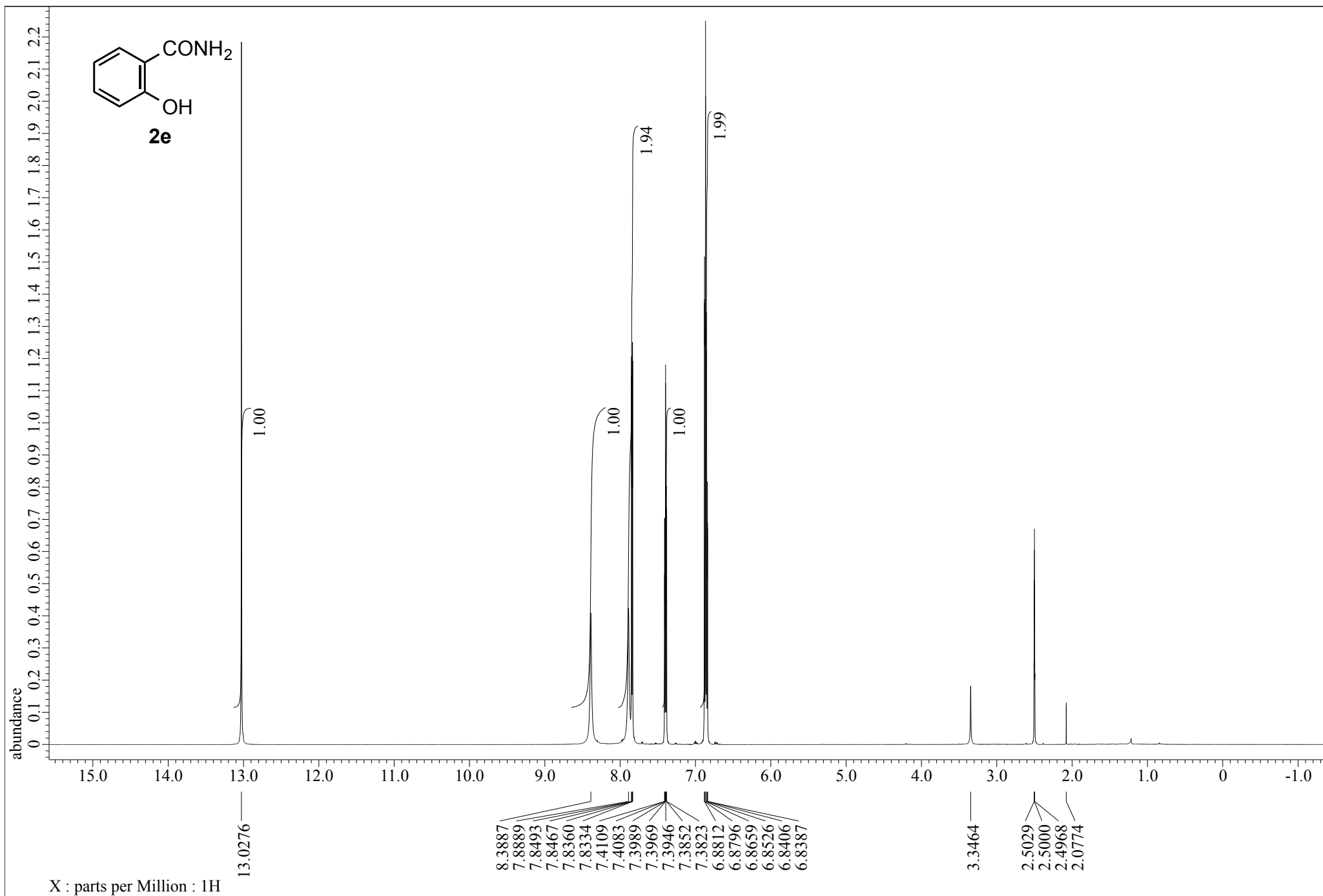


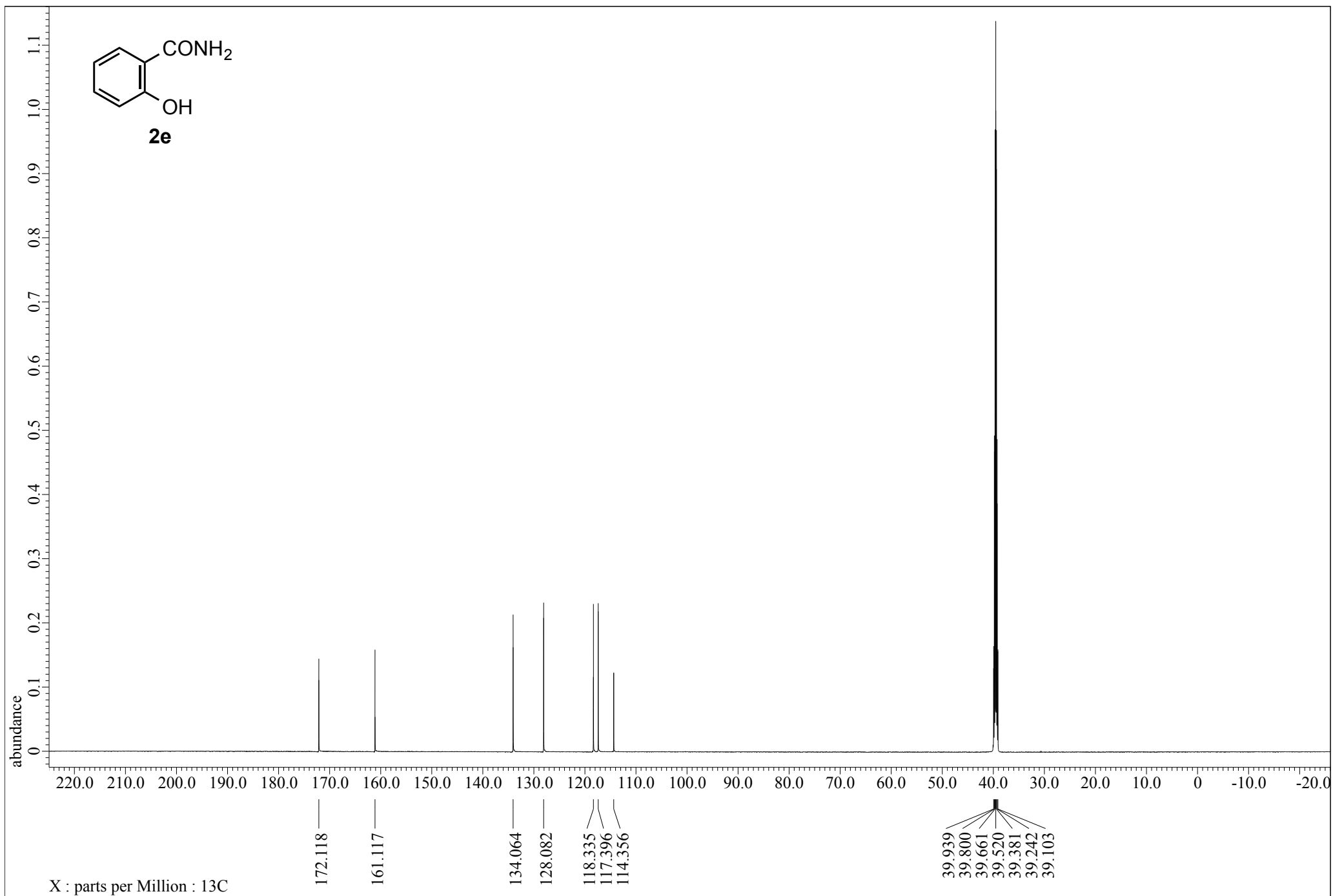
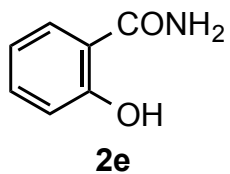


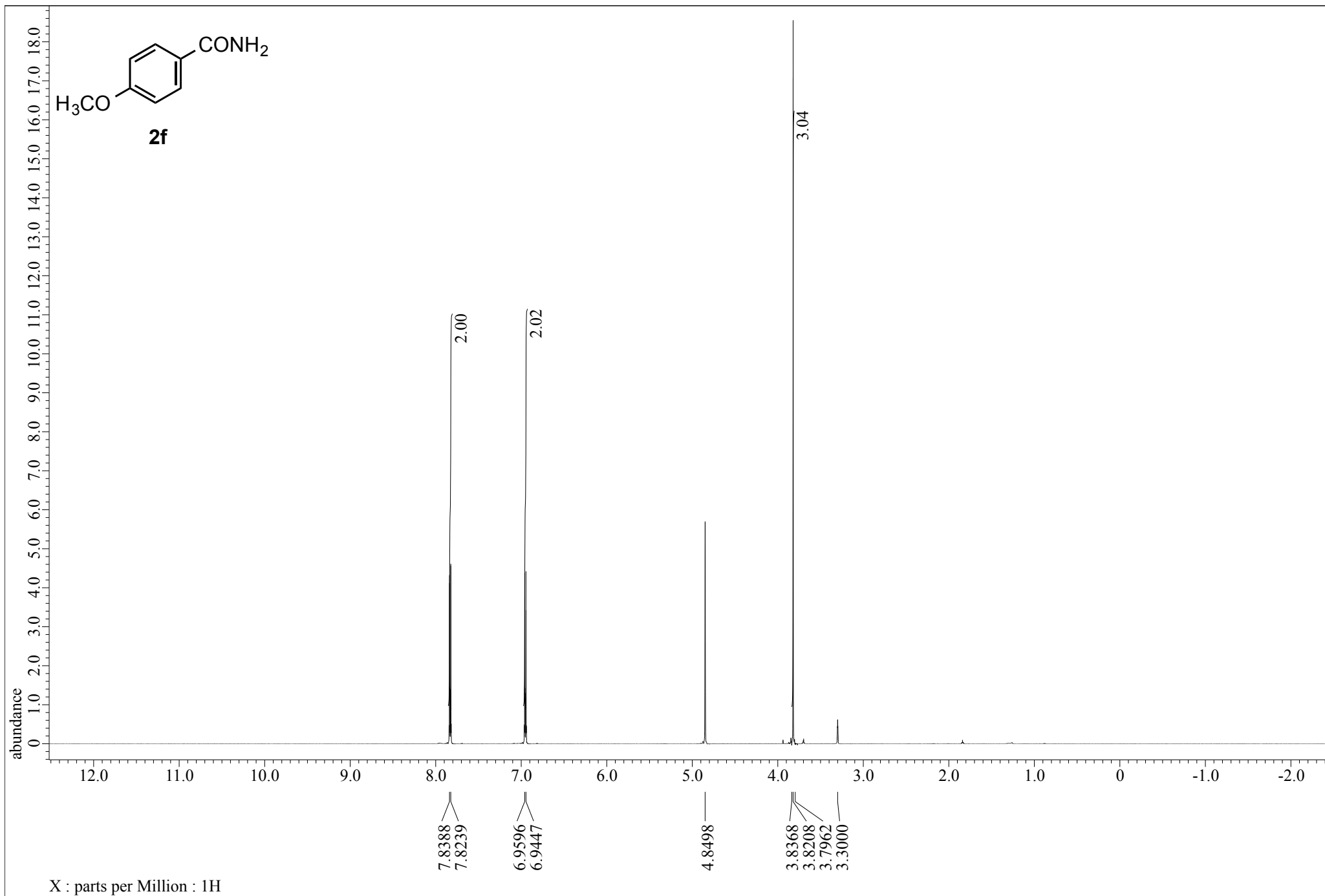


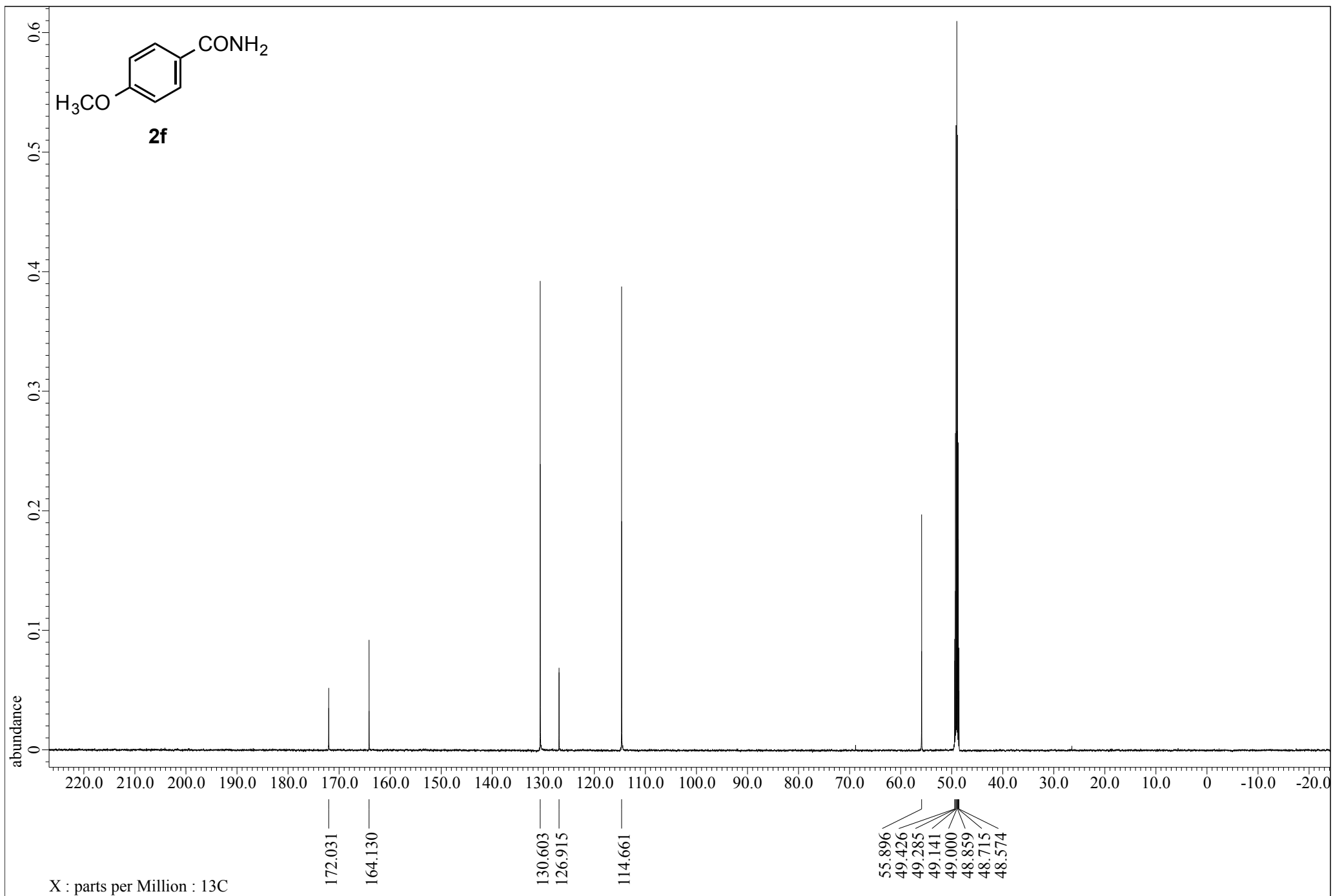


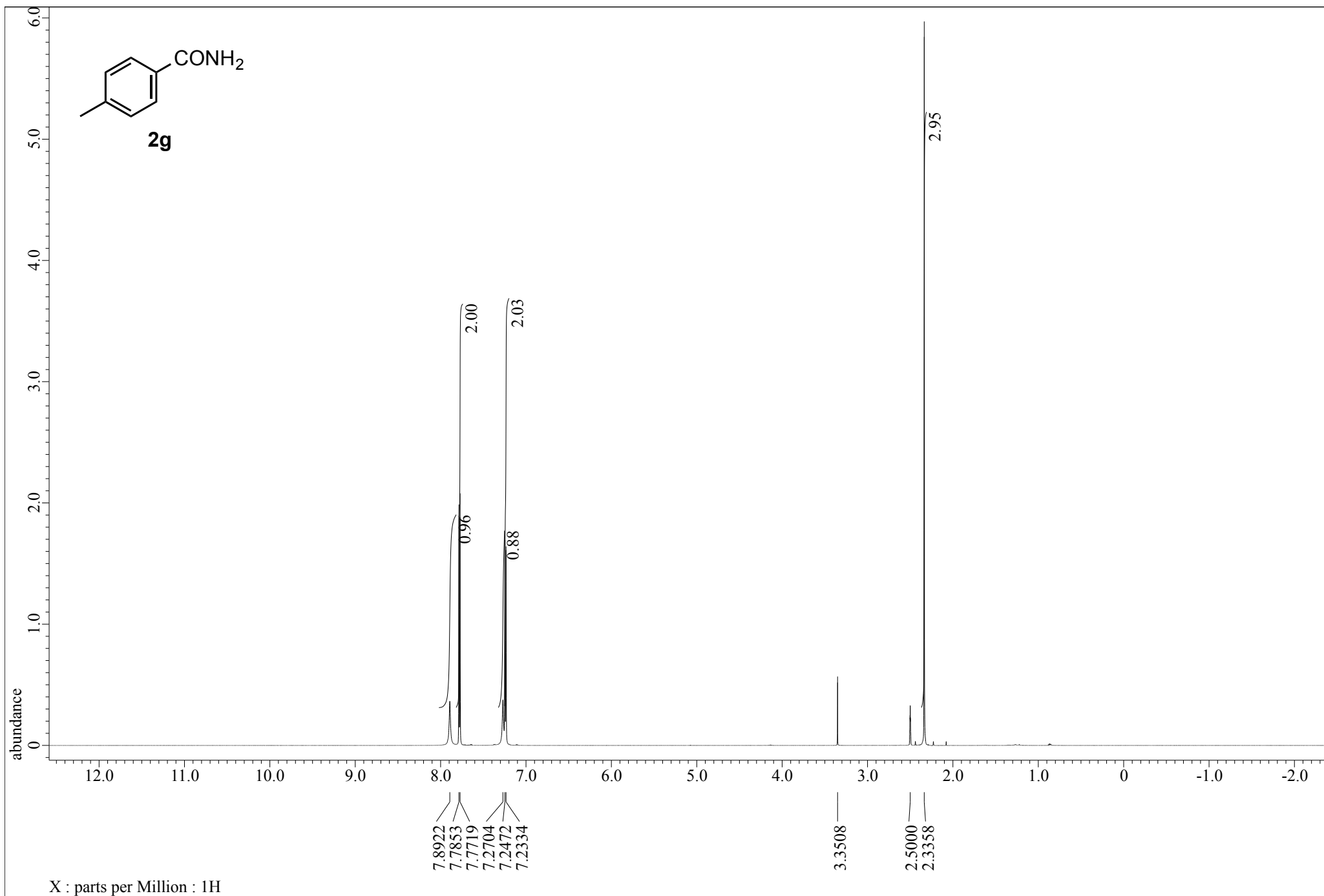


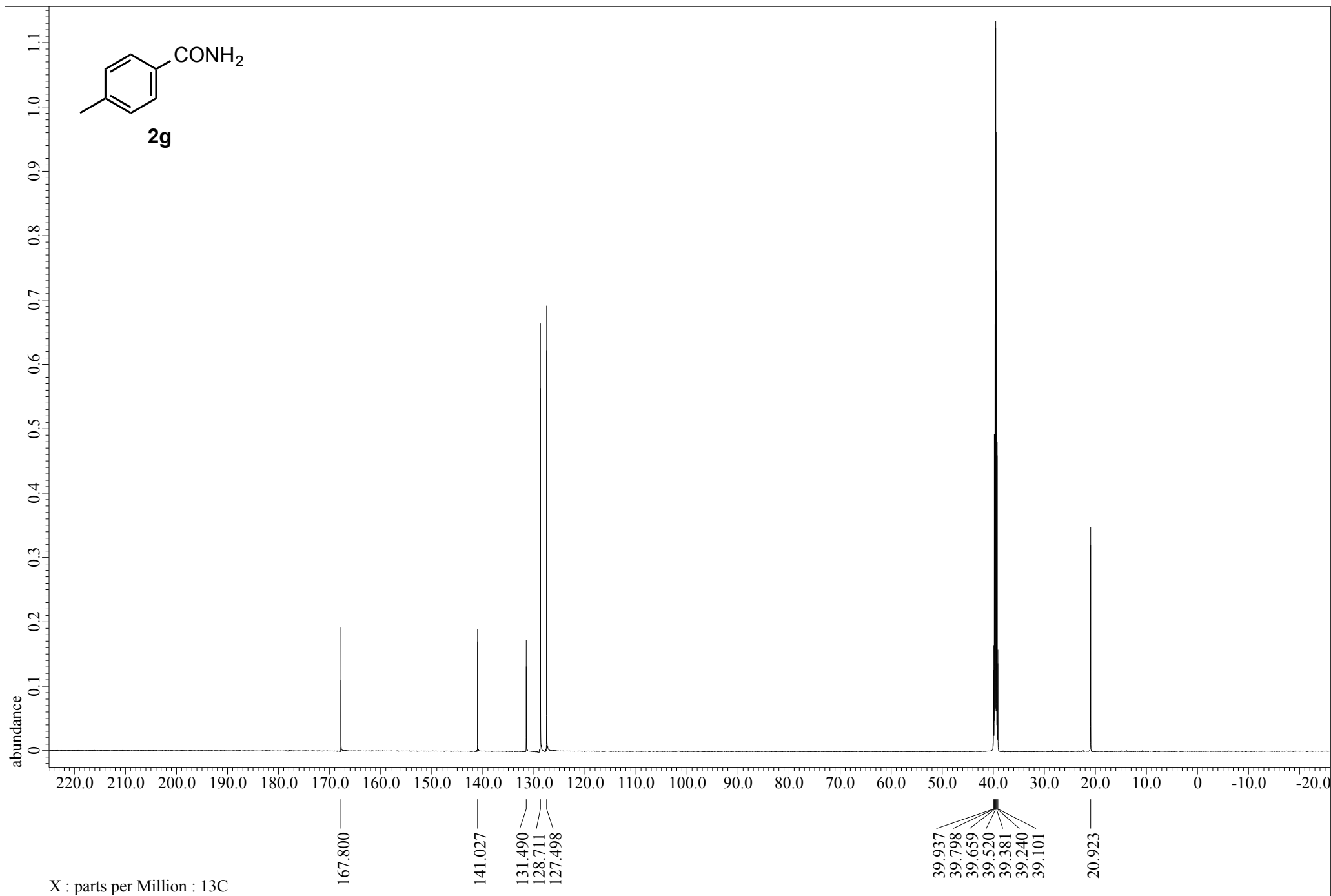


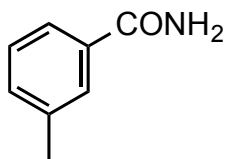




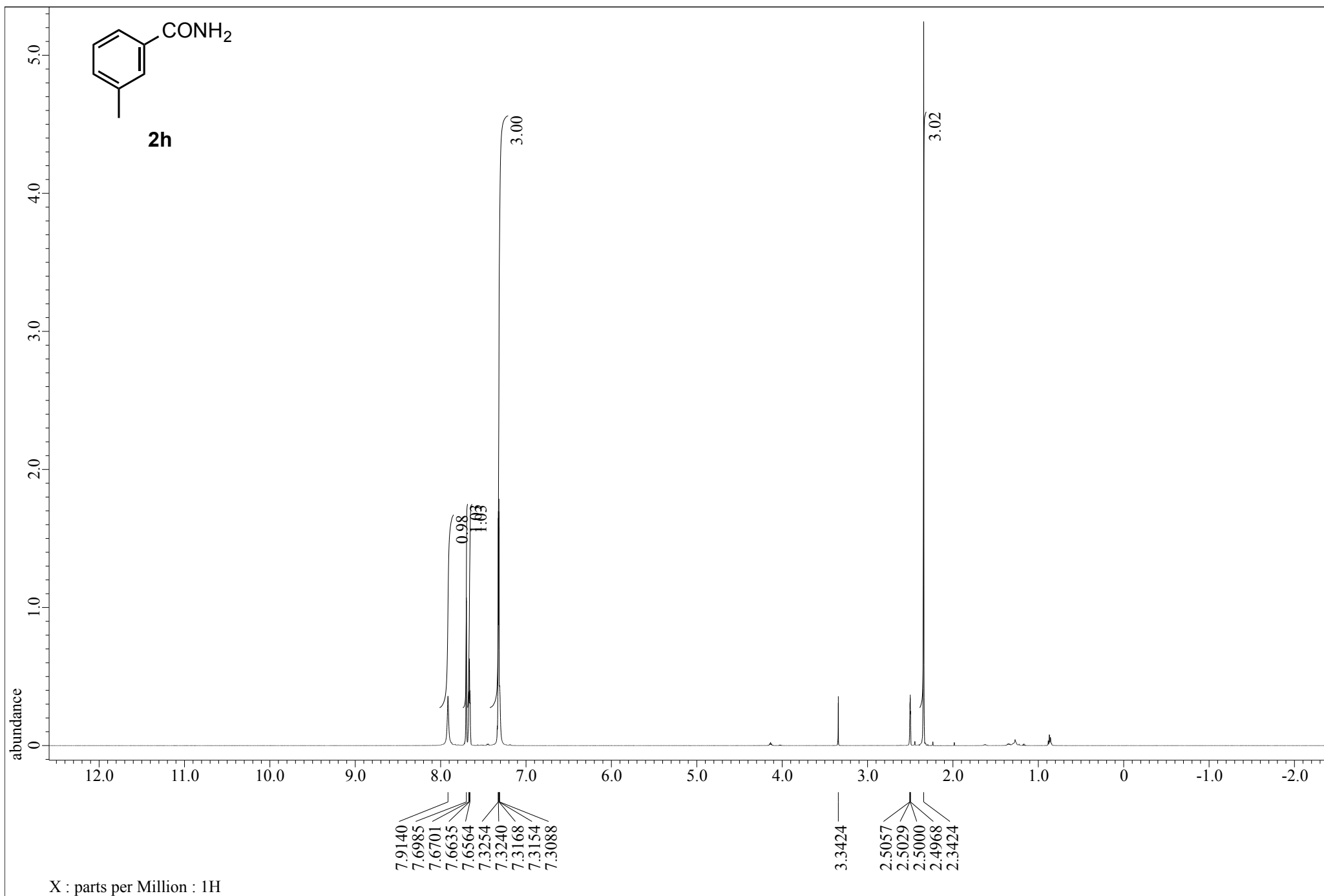


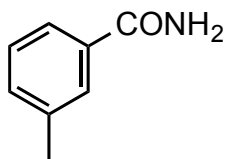




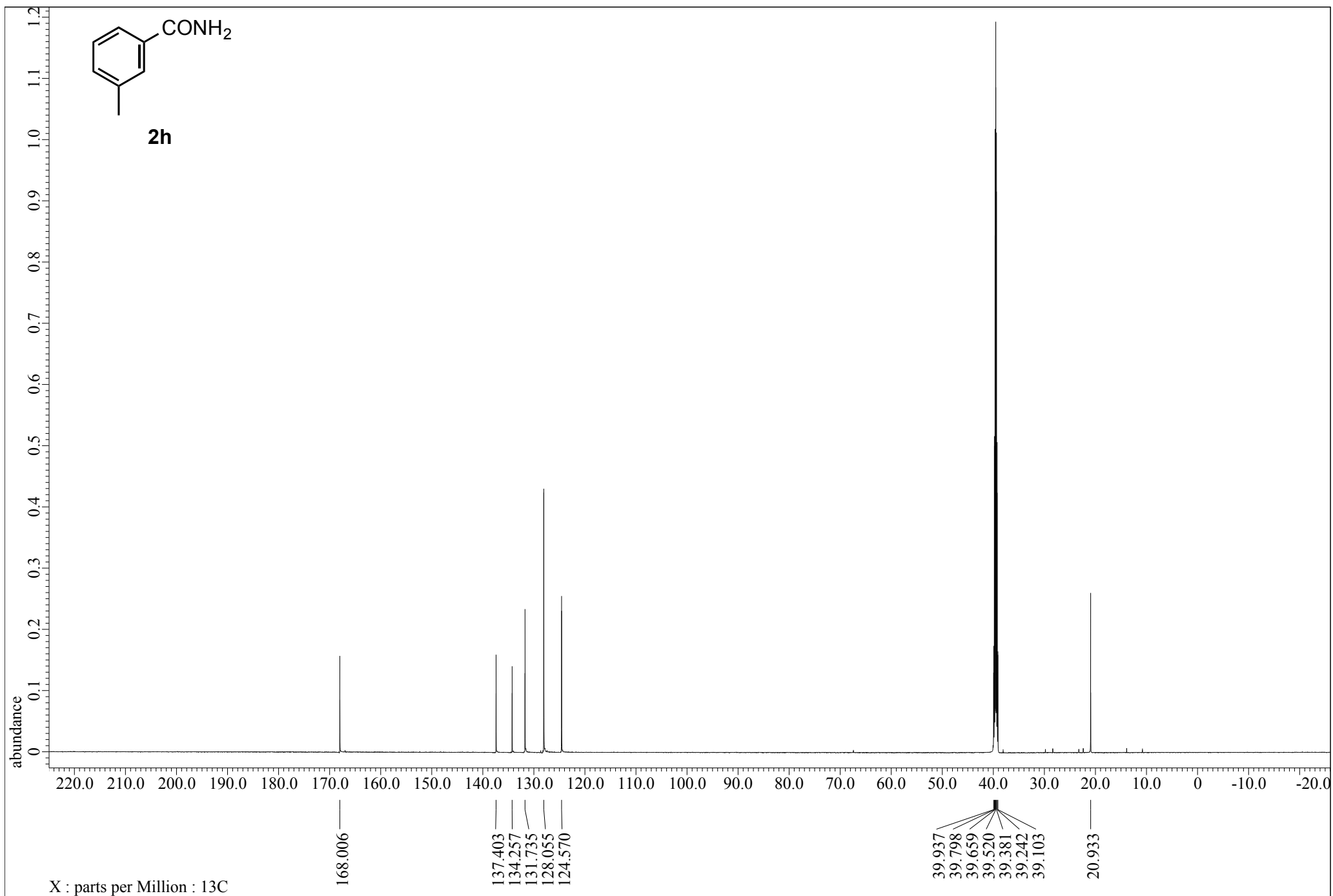


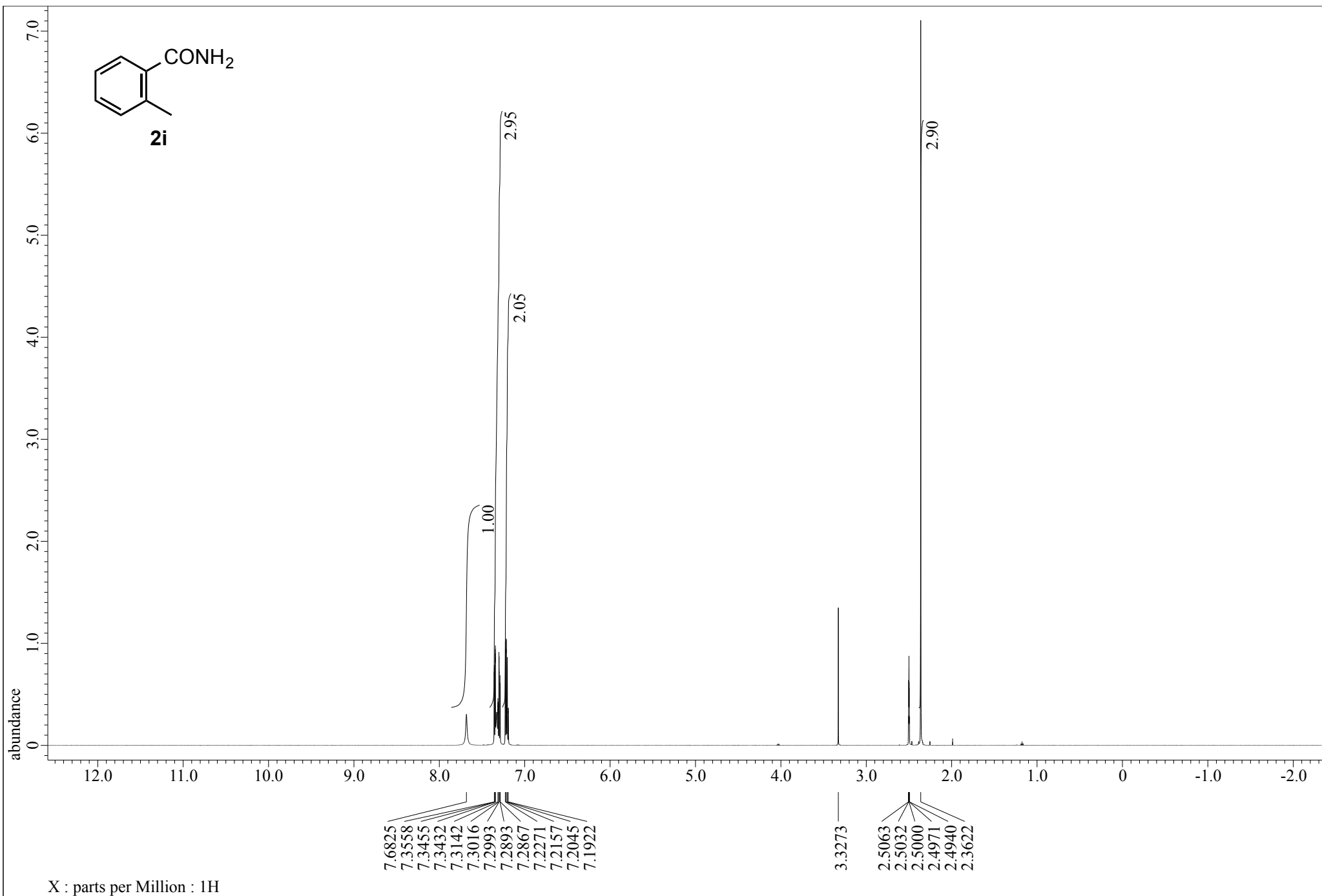
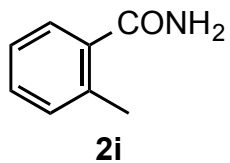
2h

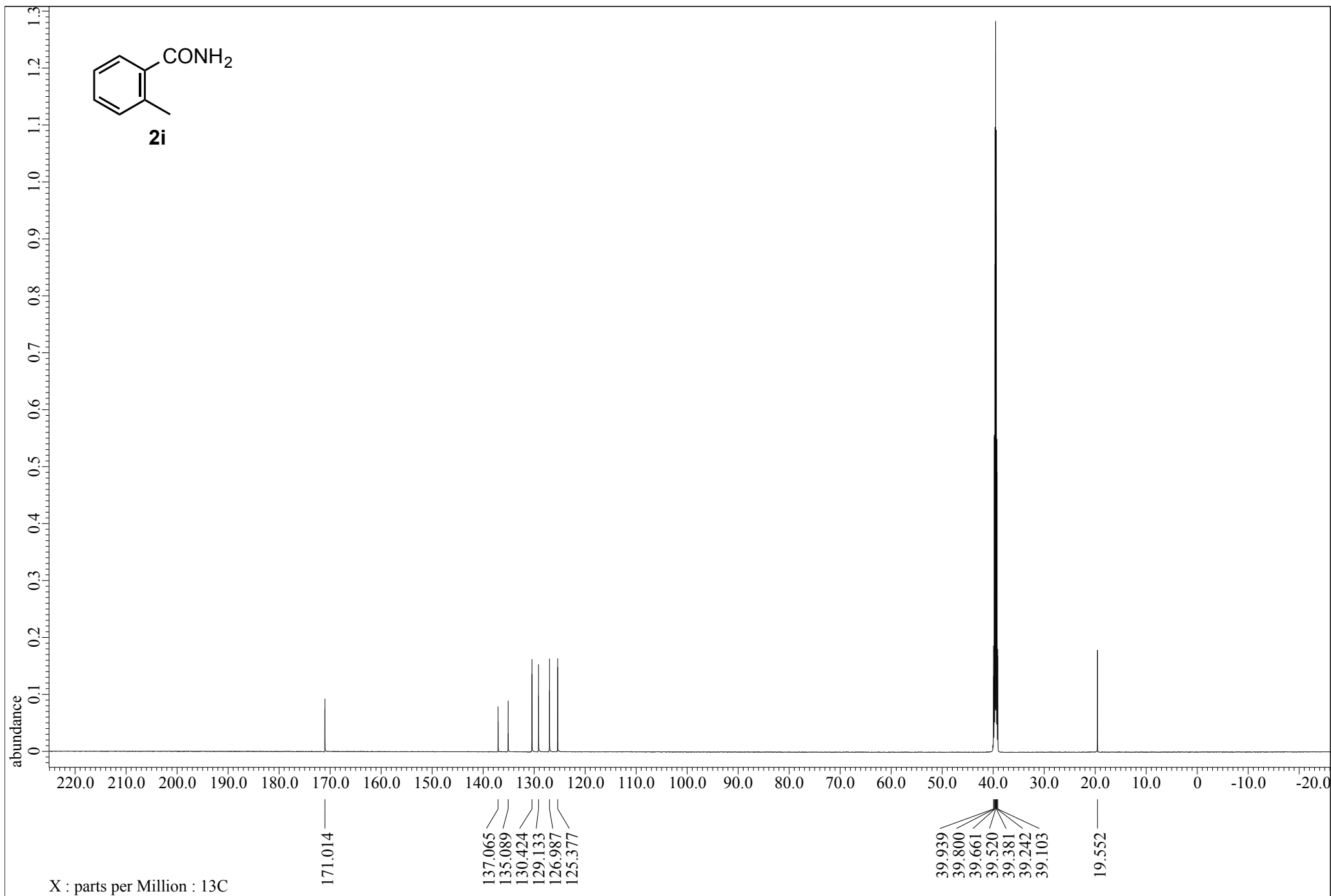
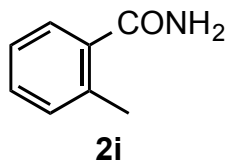


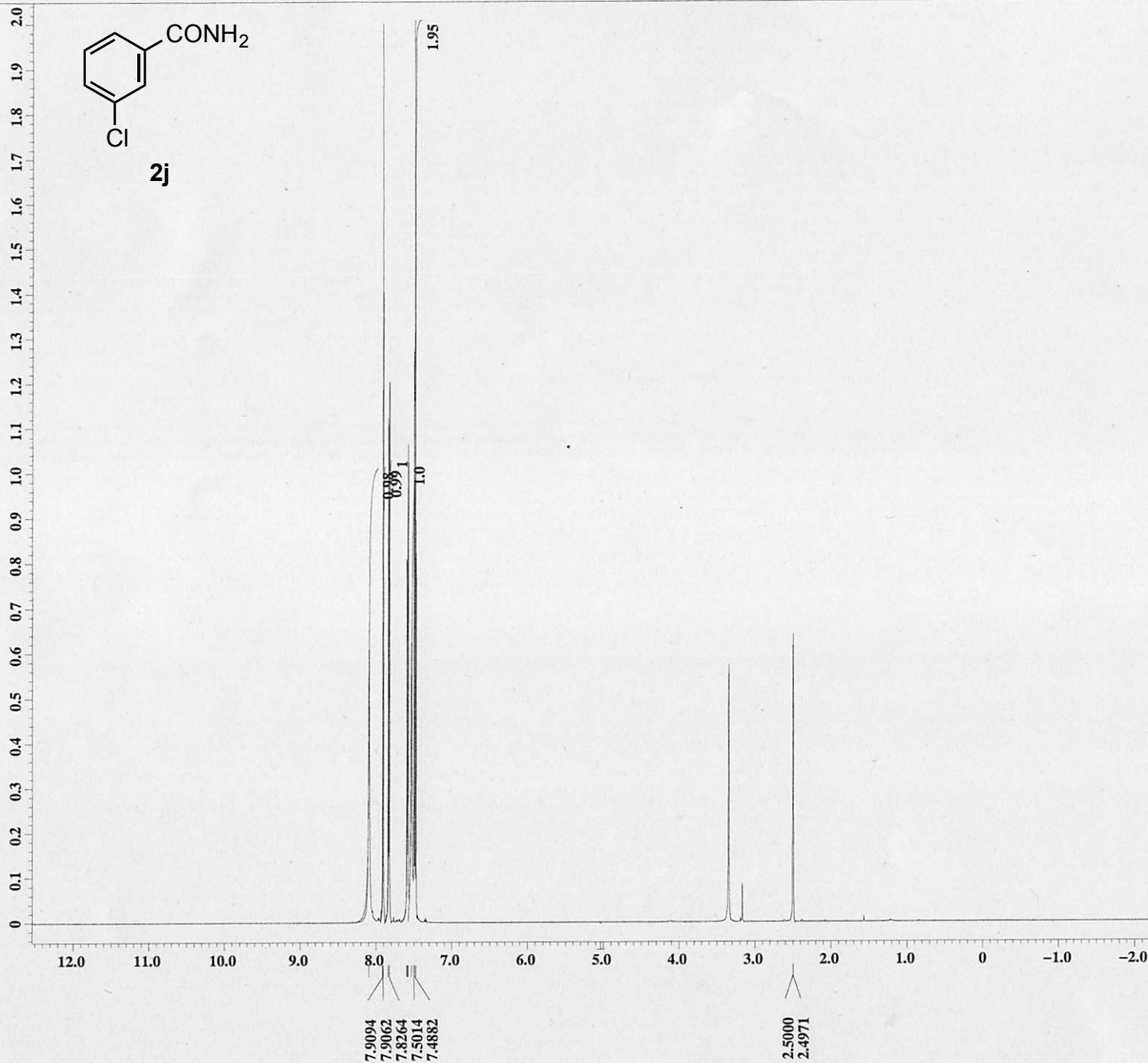


2h









X: 1H



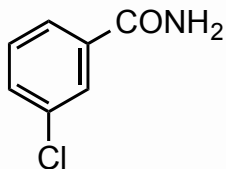
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 secp : 0.2[Hz] : 0.0[s]
 trapezoid3 : 0[%] : 80[%] : 100[%]
 zerofill : 1
 fft : 1 : TRUE : TRUE
 machinephase
 ppm
 Derived from: TI4511-a m-cl product-H-11

Filename = TI4511-a m-cl product
 Author = delta
 Experiment = single_pulse.ex2
 Sample_id = S#825066
 Solvent = DMSO-D6
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 Revision_time = 25-SEP-2014 09:53:45
 Current_time = 25-SEP-2014 09:53:51

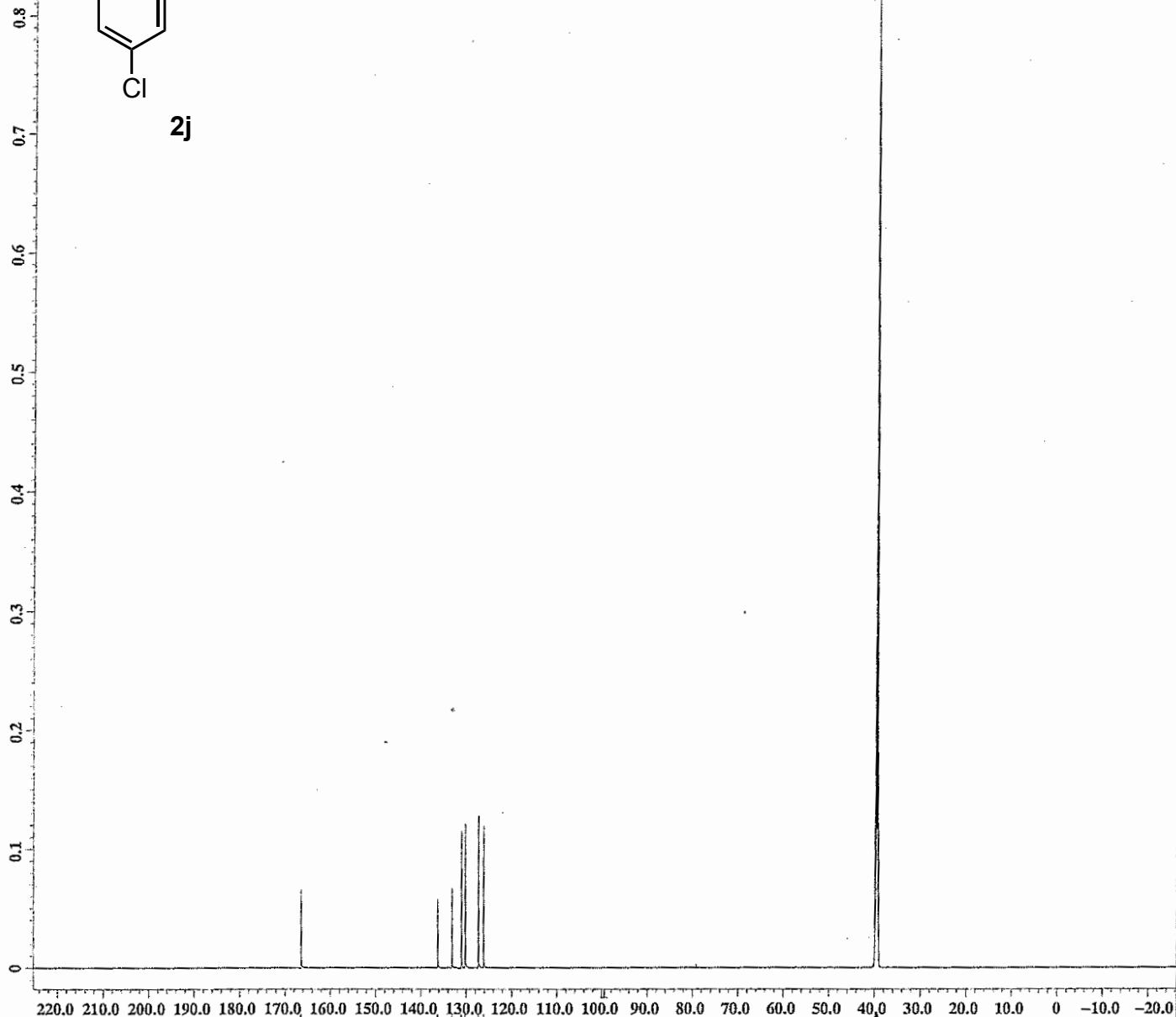
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 Dim_size = 52428
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 Dim_units = [ppm]
 Dimensions = X
 Site = ECA 600
 Spectrometer = DELTA2_NMR

Field_strength = 13.95540559[T] (590[M]
 X_acq_duration = 5.88251136[s]
 X_domain = 1H
 X_freq = 594.17058168[MHz]
 X_offset = 5[ppm]
 X_points = 65536
 X_prescans = 1
 X_resolution = 0.16999542[Hz]
 X_sweep = 11.14081996[kHz]
 Irr_domain = 1H
 Irr_freq = 594.17058168[MHz]
 Irr_offset = 5[ppm]
 Tri_domain = 1H
 Tri_freq = 594.17058168[MHz]
 Tri_offset = 5[ppm]
 Clipped = FALSE
 Mod_return = 1
 Scans = 8
 Total_scans = 8

X_90_width = 10.6[us]
 X_acq_time = 5.88251136[s]
 X_angle = 45[deg]
 X_atn = 4.9[dB]
 X_pulse = 5.3[us]
 Irr_mode = Off
 Tri_mode = Off
 Dante_presat = FALSE
 Initial_wait = 1[s]
 Recvr_gain = 40
 Relaxation_delay = 5[s]
 Repetition_time = 10.88251136[s]
 Temp_get = 22.3[dc]



2j



166.425

133.146
131.080
130.252
127.310
126.192

39.659
39.520
39.378

X: 13C

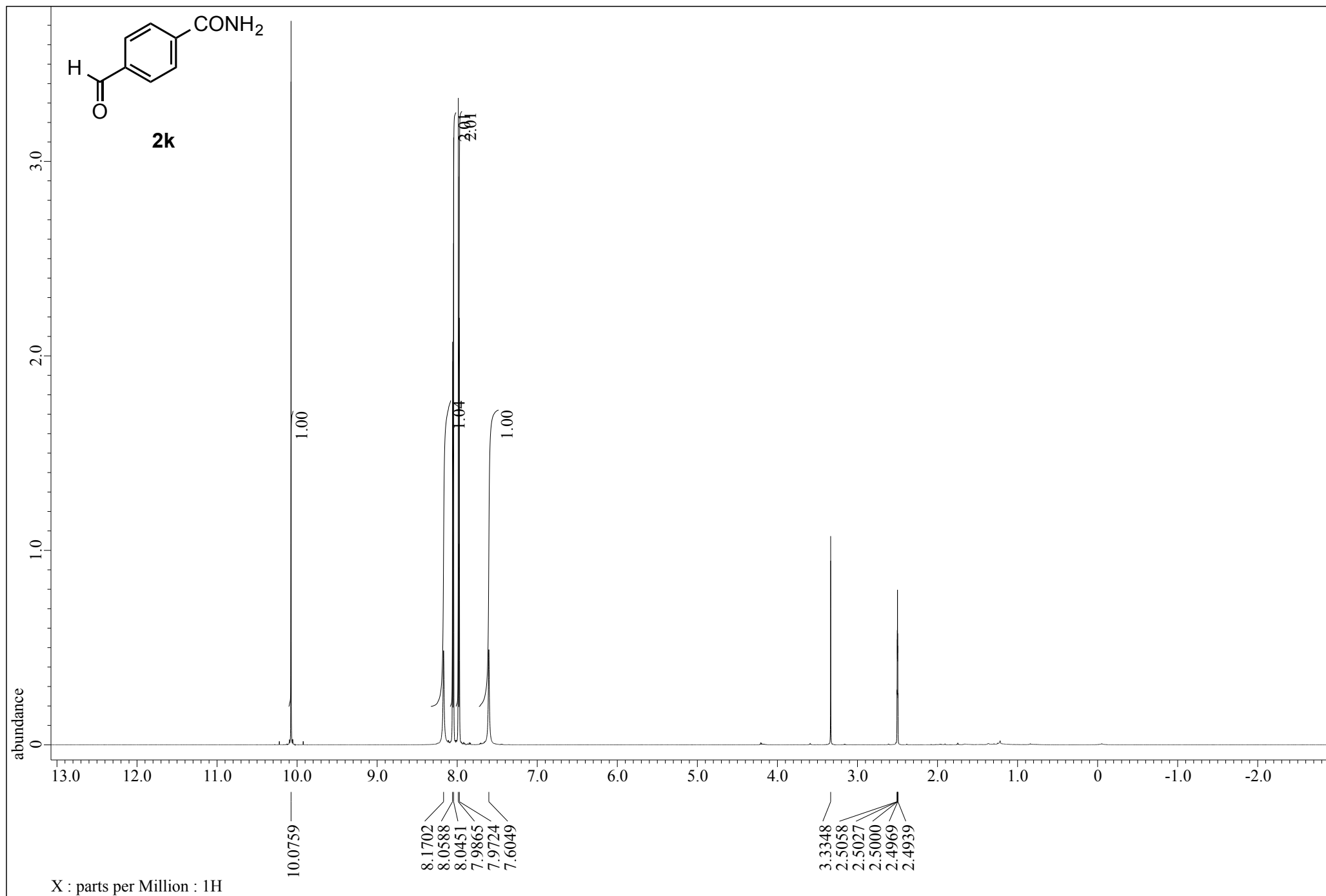


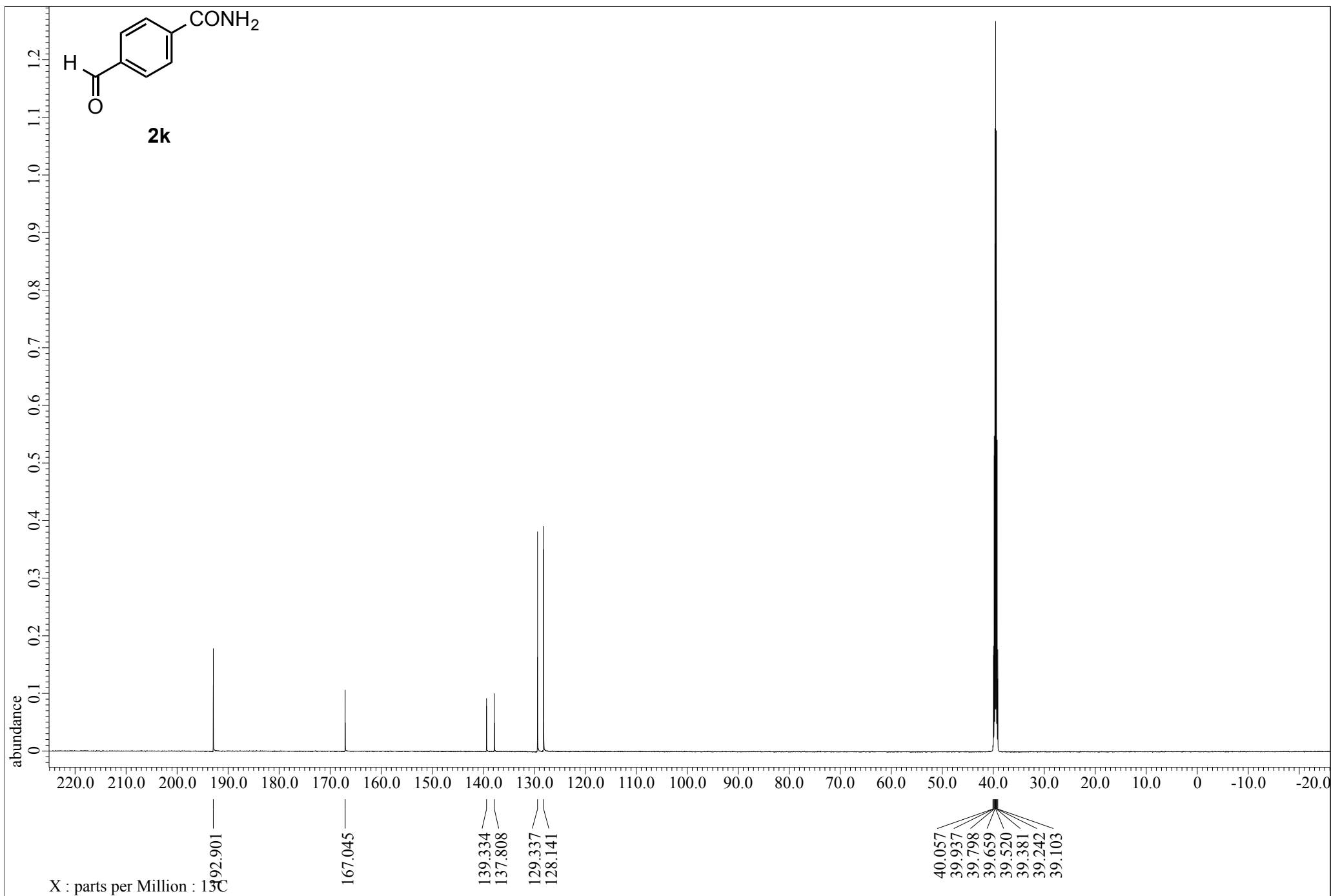
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Author = delta
Experiment = single_pulse_dec
Sample_id = S#829126
Solvent = DMSO-D6
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Revision_time = 13-AUG-2014 16:38:06
Current_time = 18-AUG-2014 18:53:40

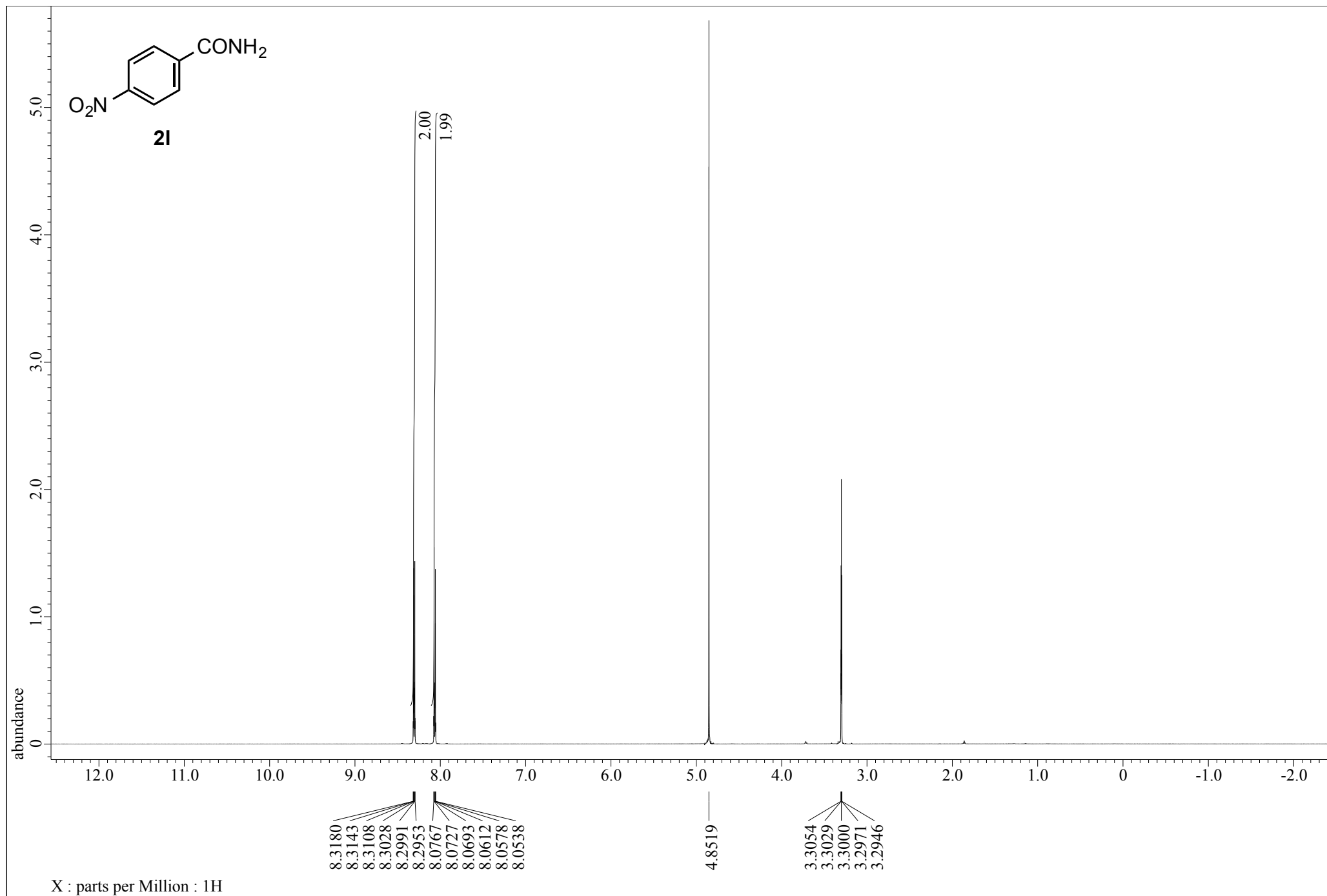
Comment = single pulse decouple
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Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA 600
Spectrometer = DELTA2_NMR

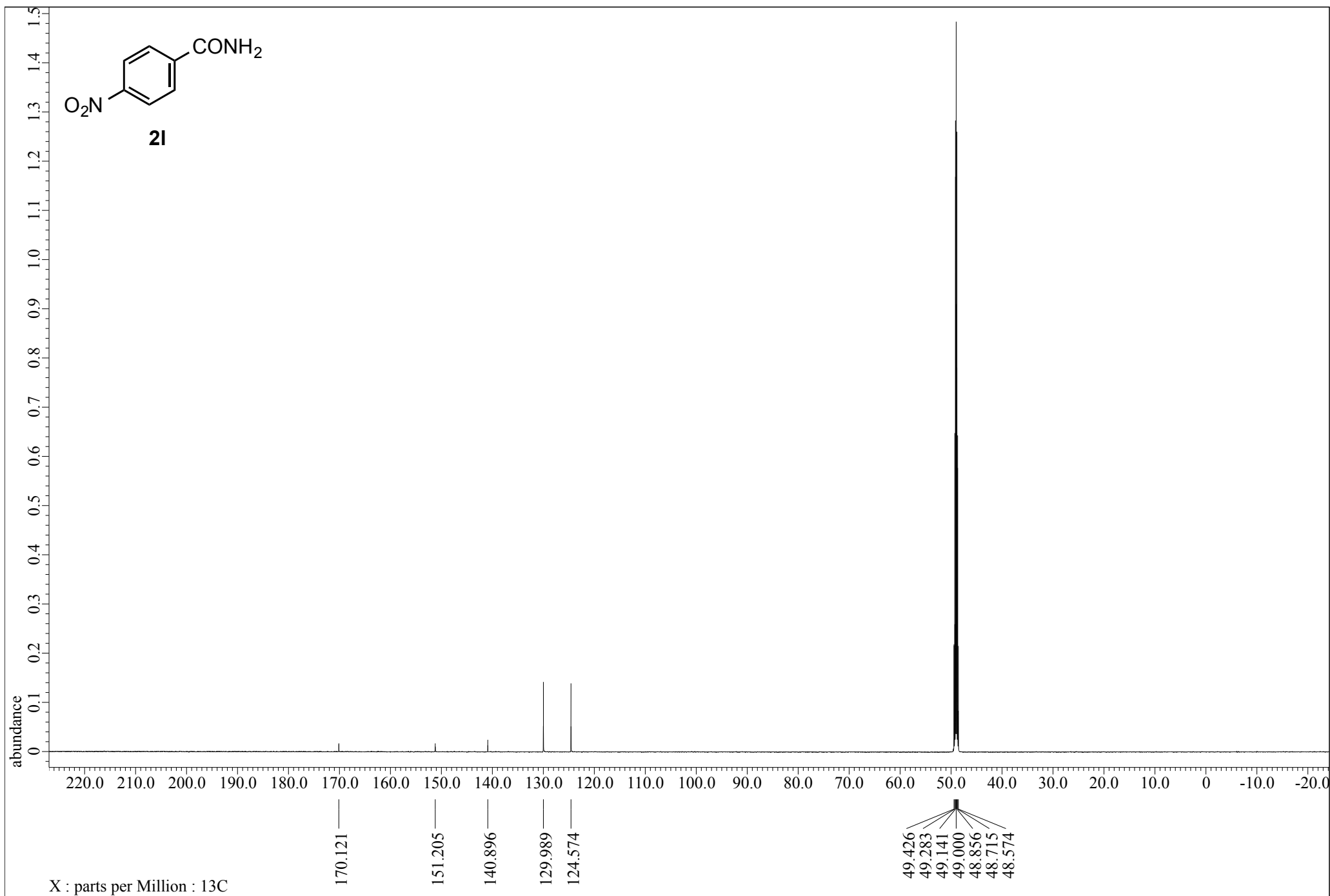
Field_strength = 13.95540559 [T] (590 [M]
X_acq_duration = 2.78921216 [s]
X_domain = 13C
X_freq = 149.40429612 [MHz]
X_offset = 100 [ppm]
X_points = 131072
X_prescans = 4
X_resolution = 0.35852418 [Hz]
X_sweep = 46.9924812 [kHz]
Irr_domain = 1H
Irr_freq = 594.17058168 [MHz]
Irr_offset = 5 [ppm]
Clipped = FALSE
Mod_return = 1
Scans = 8012
Total_scans = 8012

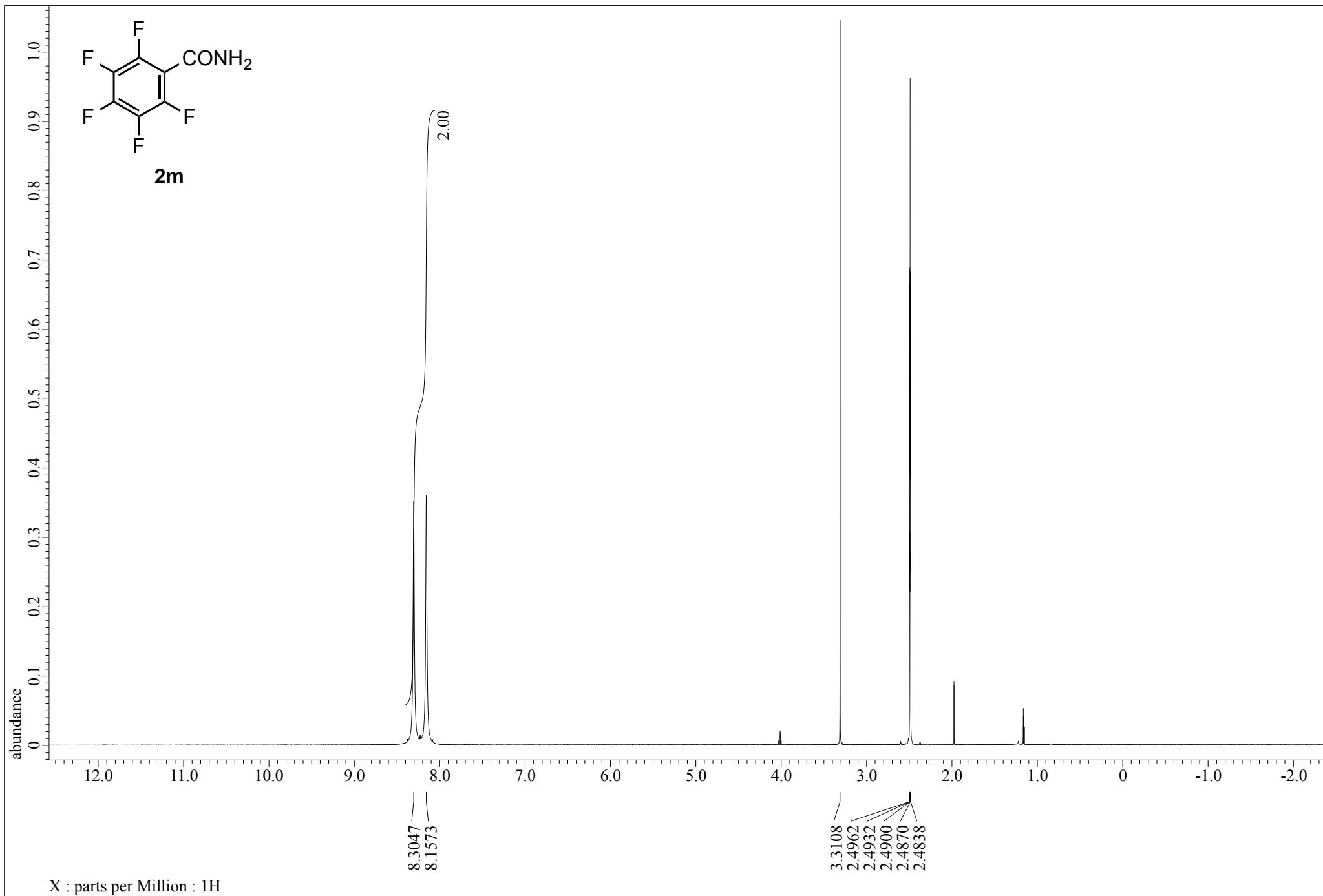
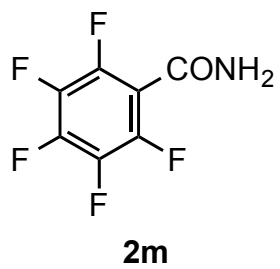
X_90_width = 8.6 [us]
X_acq_time = 2.78921216 [s]
X_angle = 30 [deg]
X_atn = 6.9 [dB]
X_pulse = 2.86666667 [us]
Irr_atn_dec = 22.01015 [dB]
Irr_atn_noe = 22.01015 [dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1 [s]
Noe = TRUE
Noe_time = 2 [s]
Recvr_gain = 56
Relaxation_delay = 2 [s]
Repetition_time = 4.78921216 [s]
Temp_get = 23 [dc]

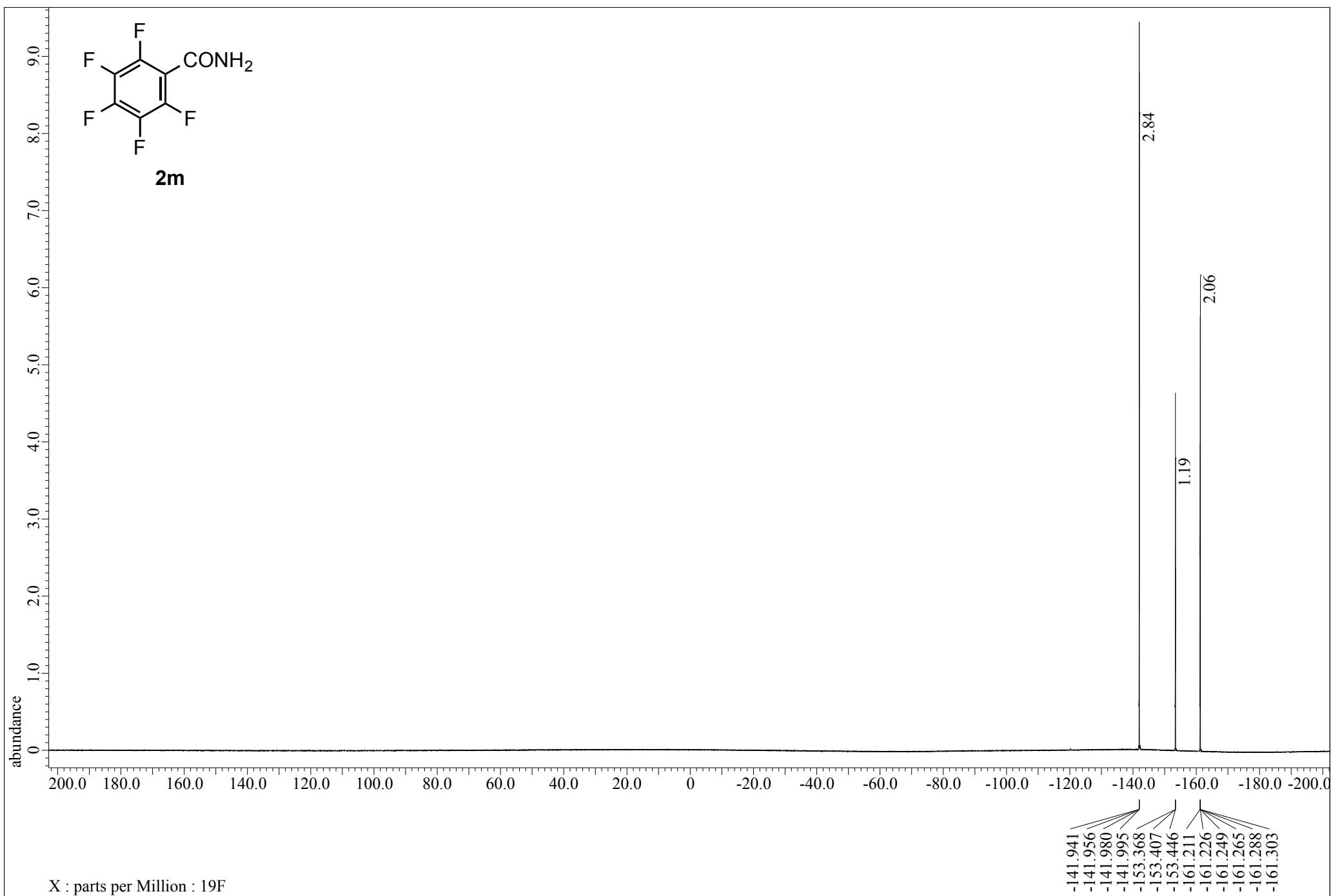
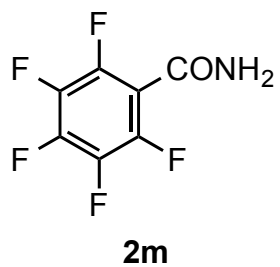


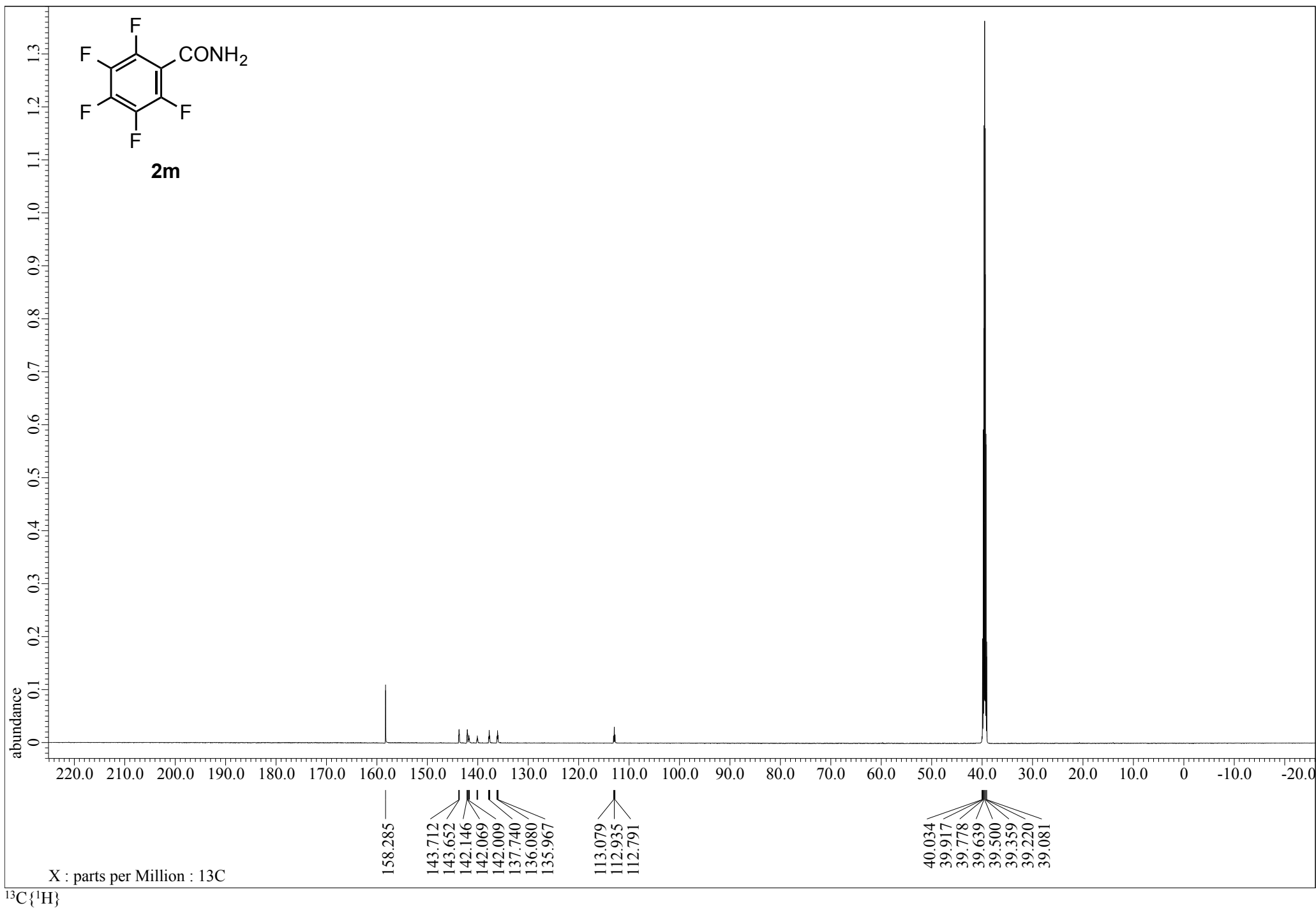




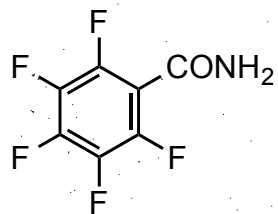




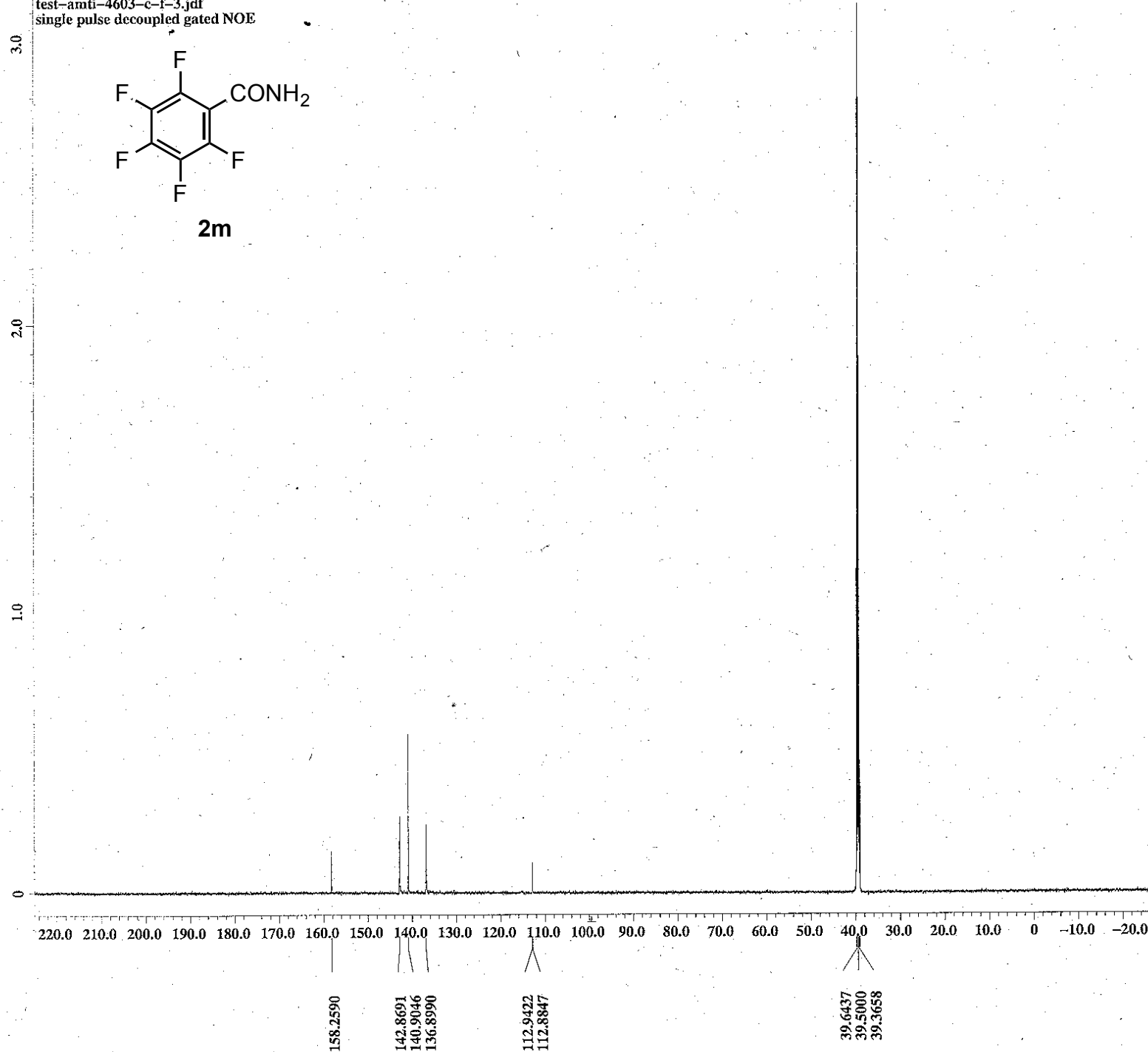




$^{13}\text{C}\{^1\text{H}\}$



2m



X : parts per Million : 13C



----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
semp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

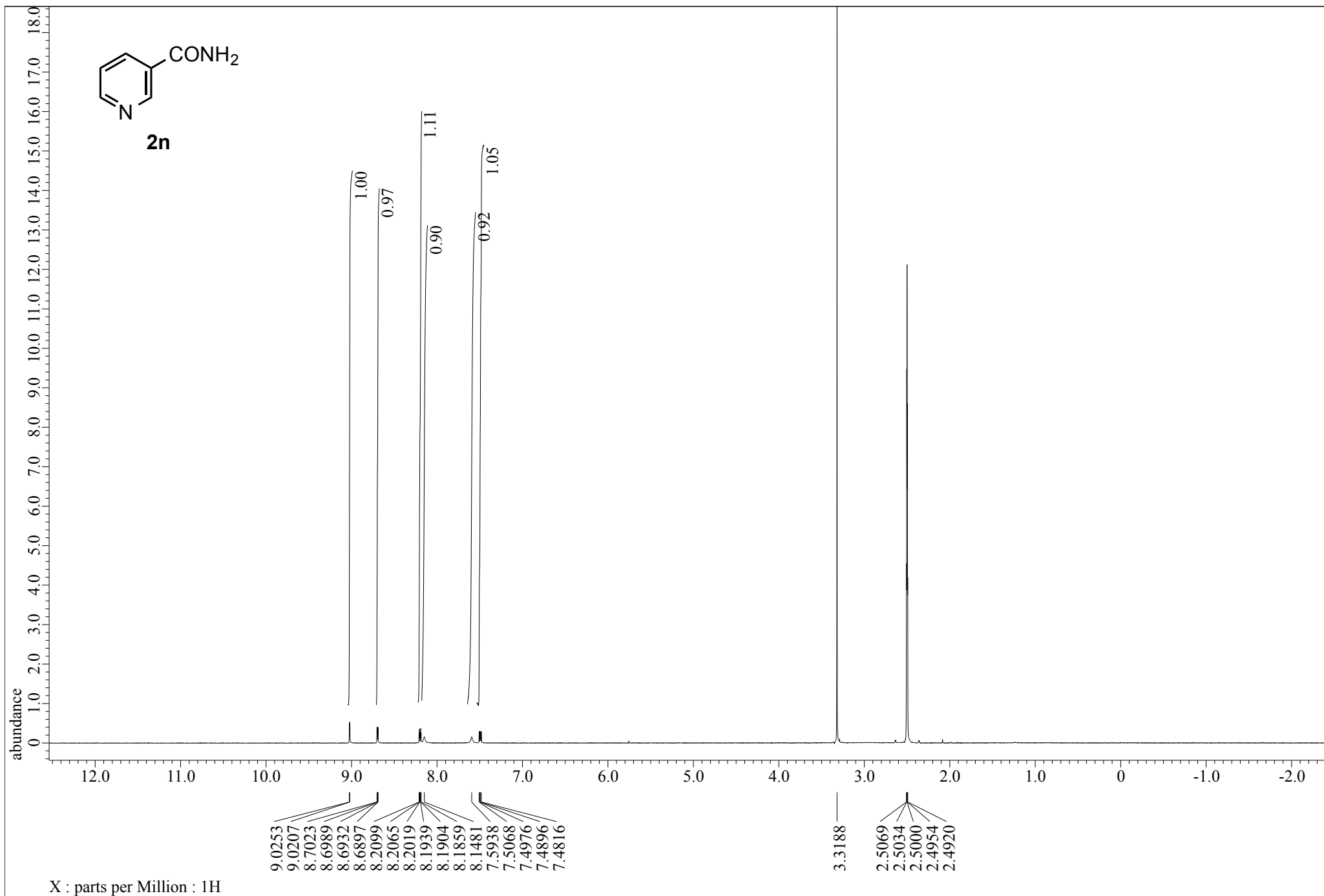
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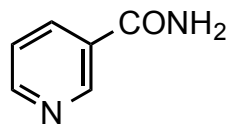
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Author = noyori
Experiment = single_pulse_dec
Sample_id = S#282820
Solvent = DMSO-D6
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Revision_time = 10-SEP-2014 08:50:02
Current_time = 10-SEP-2014 08:50:40

Content = single pulse decouple
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Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECA600
Spectrometer = JNM-ECA600

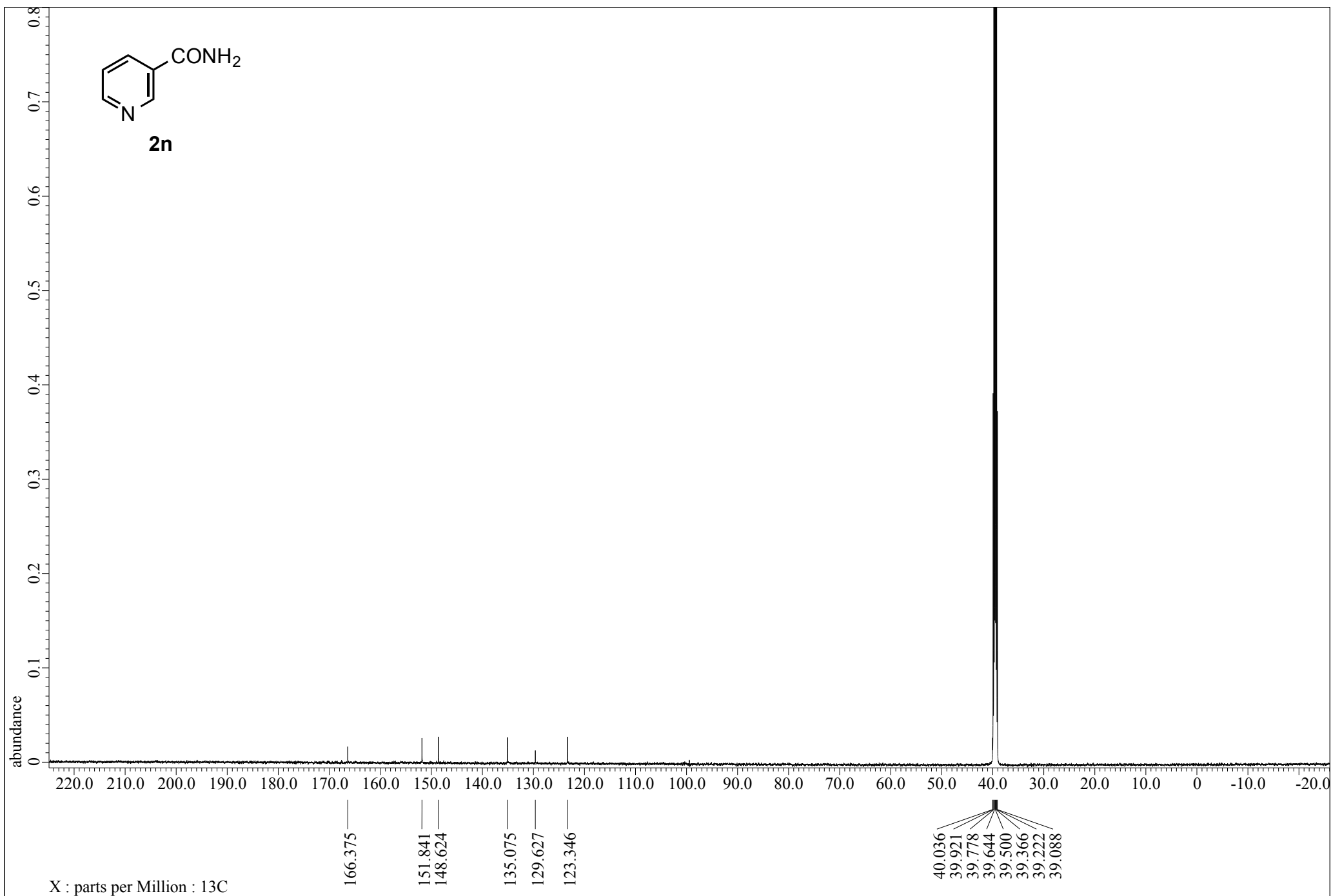
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X_domain = 13C
X_freq = 150.78770543[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 1.44496109[Hz]
X_sweep = 47.34848485[kHz]
Irr_domain = 19F
Irr_freq = 564.25564705[MHz]
Irr_offset = -152[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1000
Total_scans = 1000

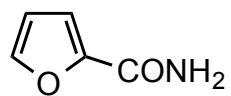
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X_acq_time = 0.69206016[s]
X_angle = 30[deg]
X_atn = 7.8[db]
X_pulse = 3.86666667[us]
Irr_atn_dec = 16.041[db]
Irr_atn_noe = 16.041[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 2.69206016[s]
Temp_get = 26.7[dc]



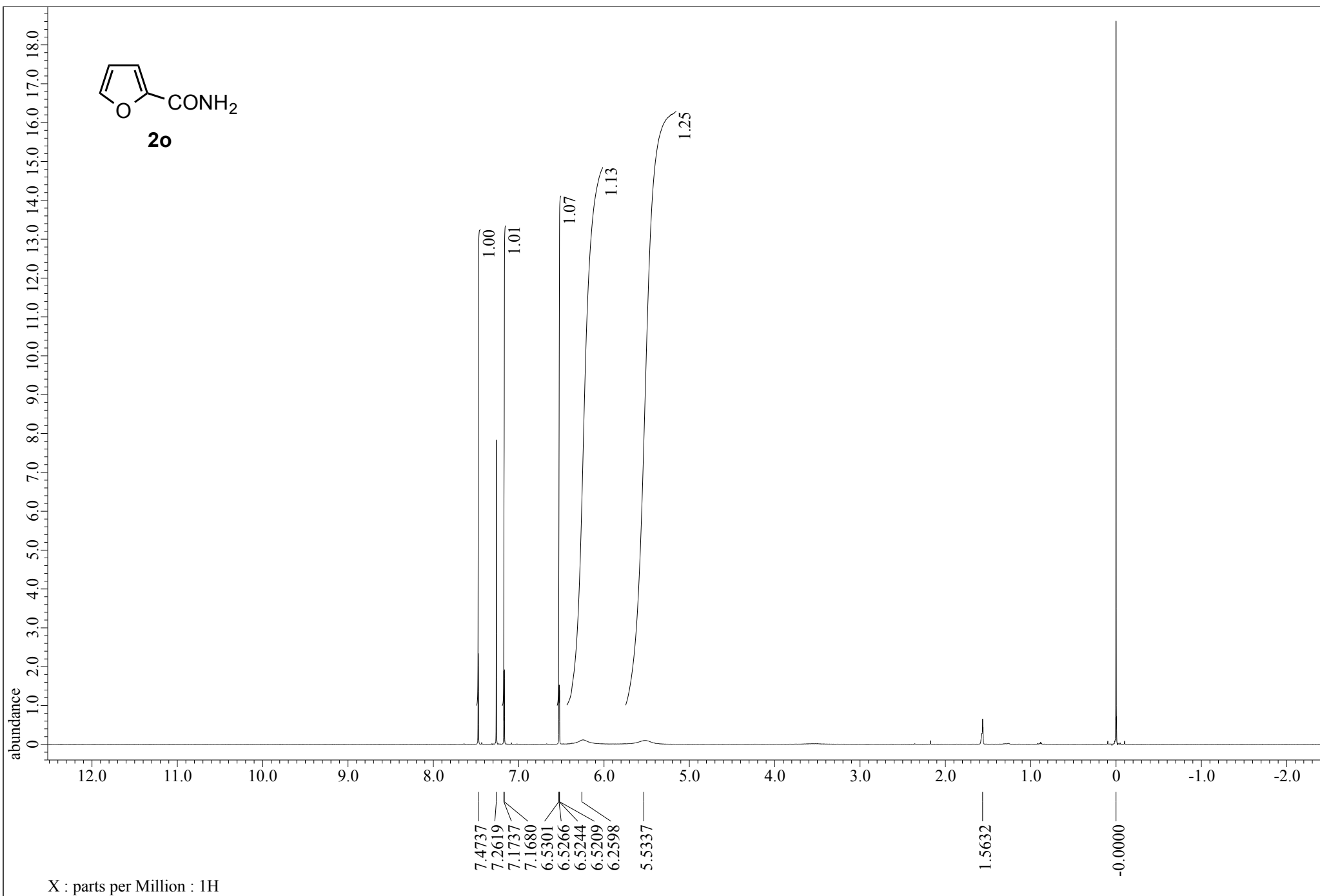


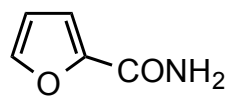
2n



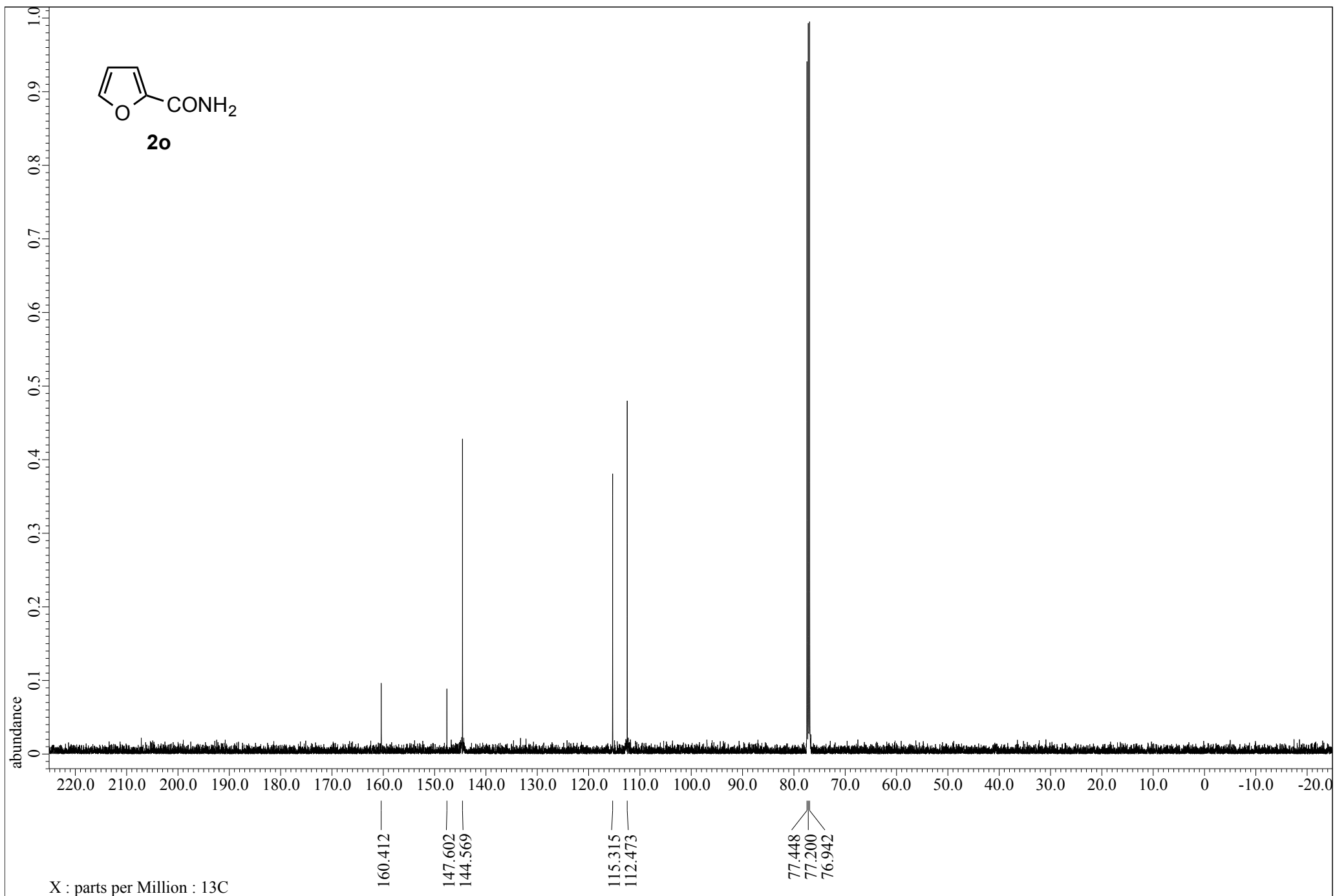


2o



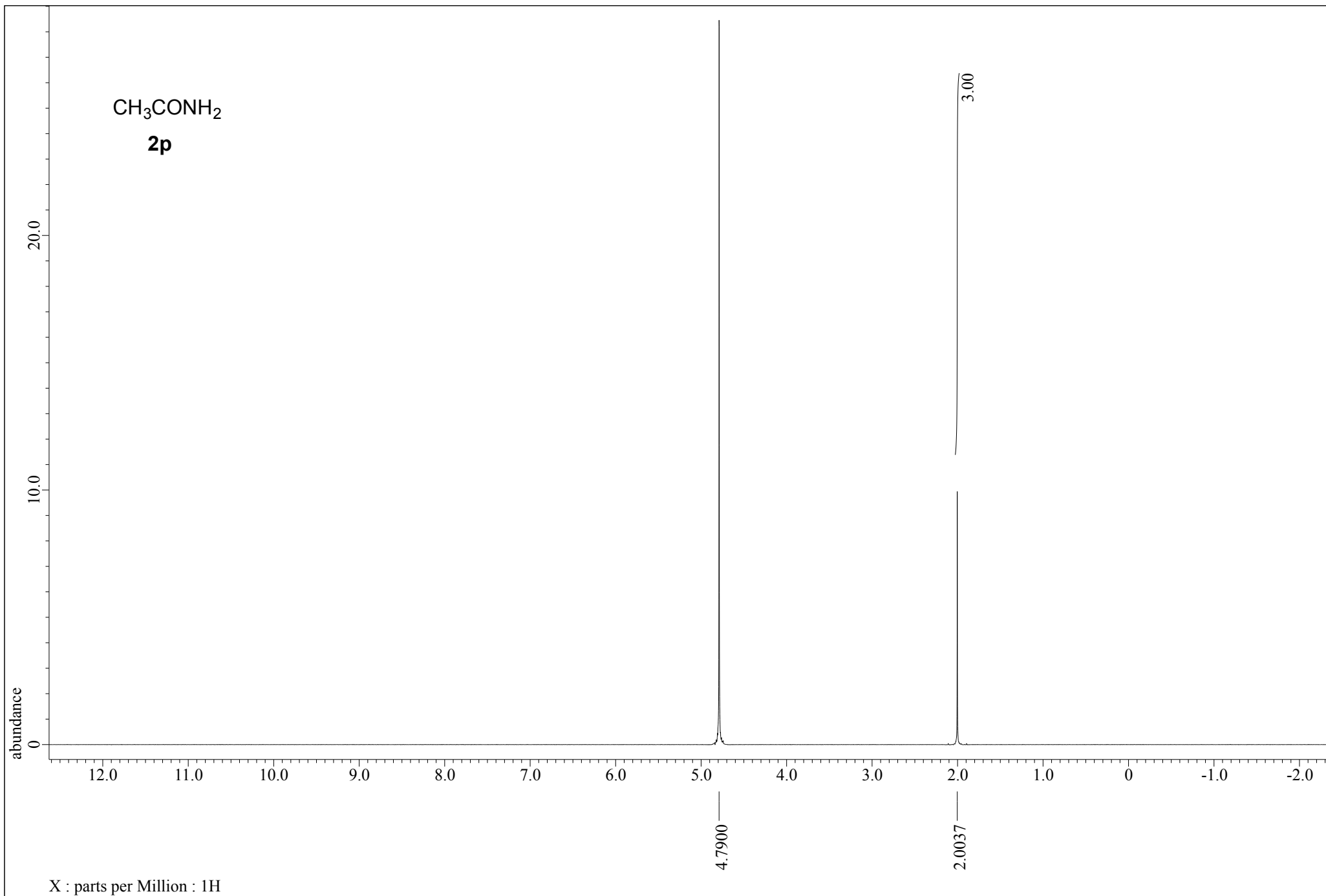


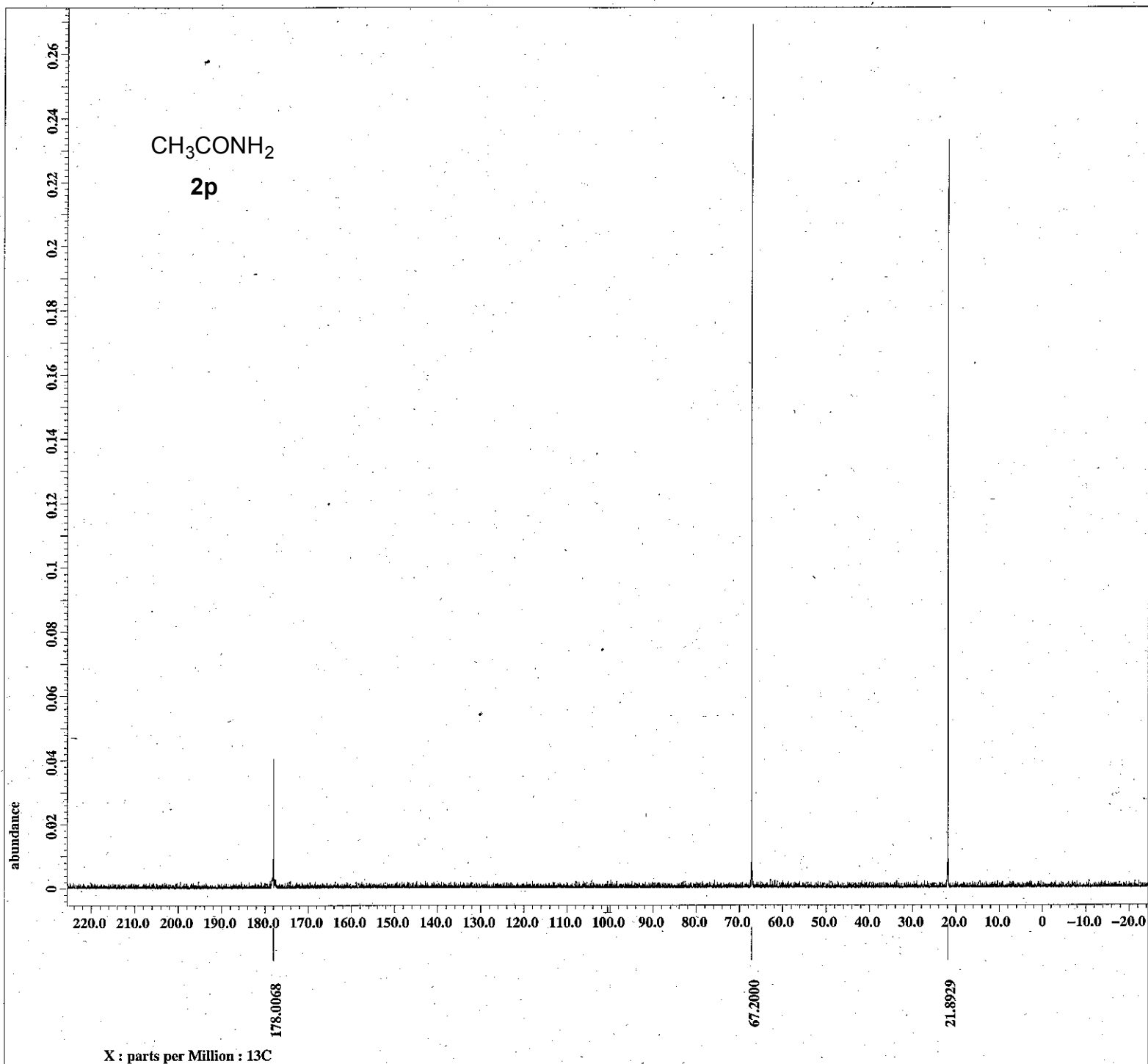
2o



CH₃CONH₂

2p





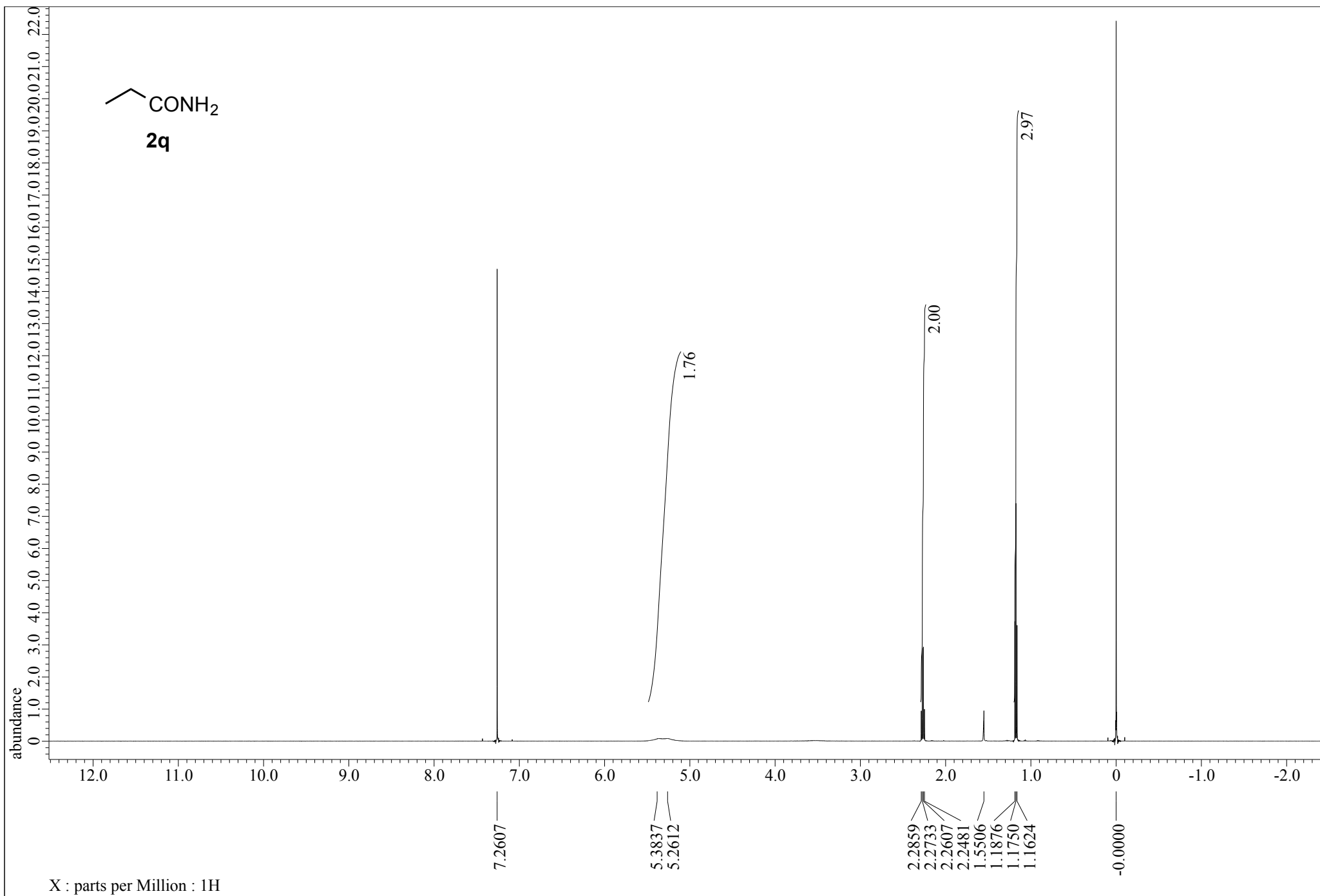
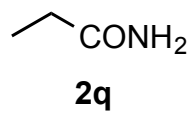
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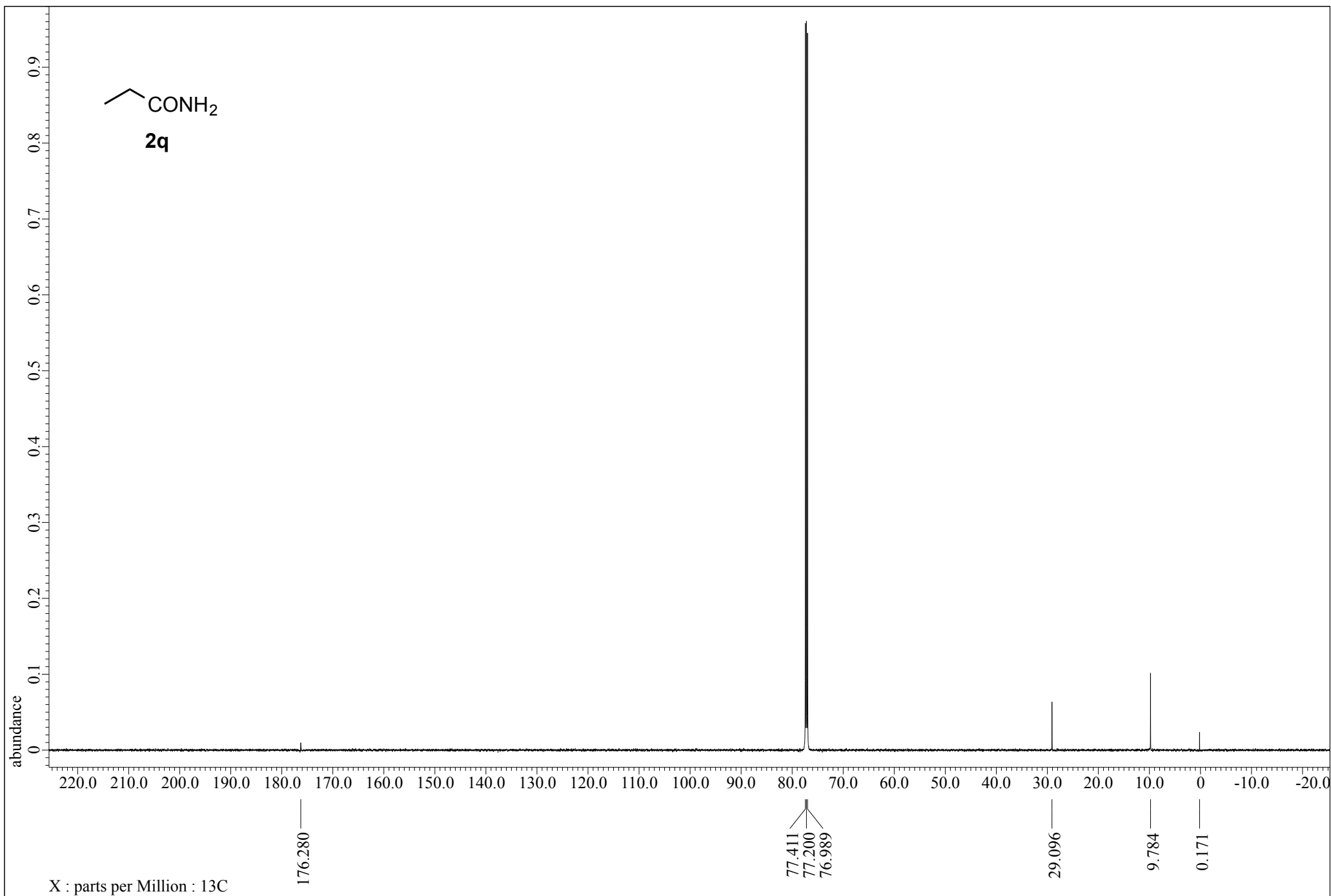
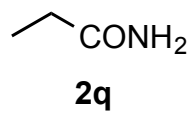
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Author       = noyori
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Sample_id    = S#837453
Solvent      = D2O
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Revision_time = 9-SEP-2014 08:48:53
Current_time  = 9-SEP-2014 08:49:07

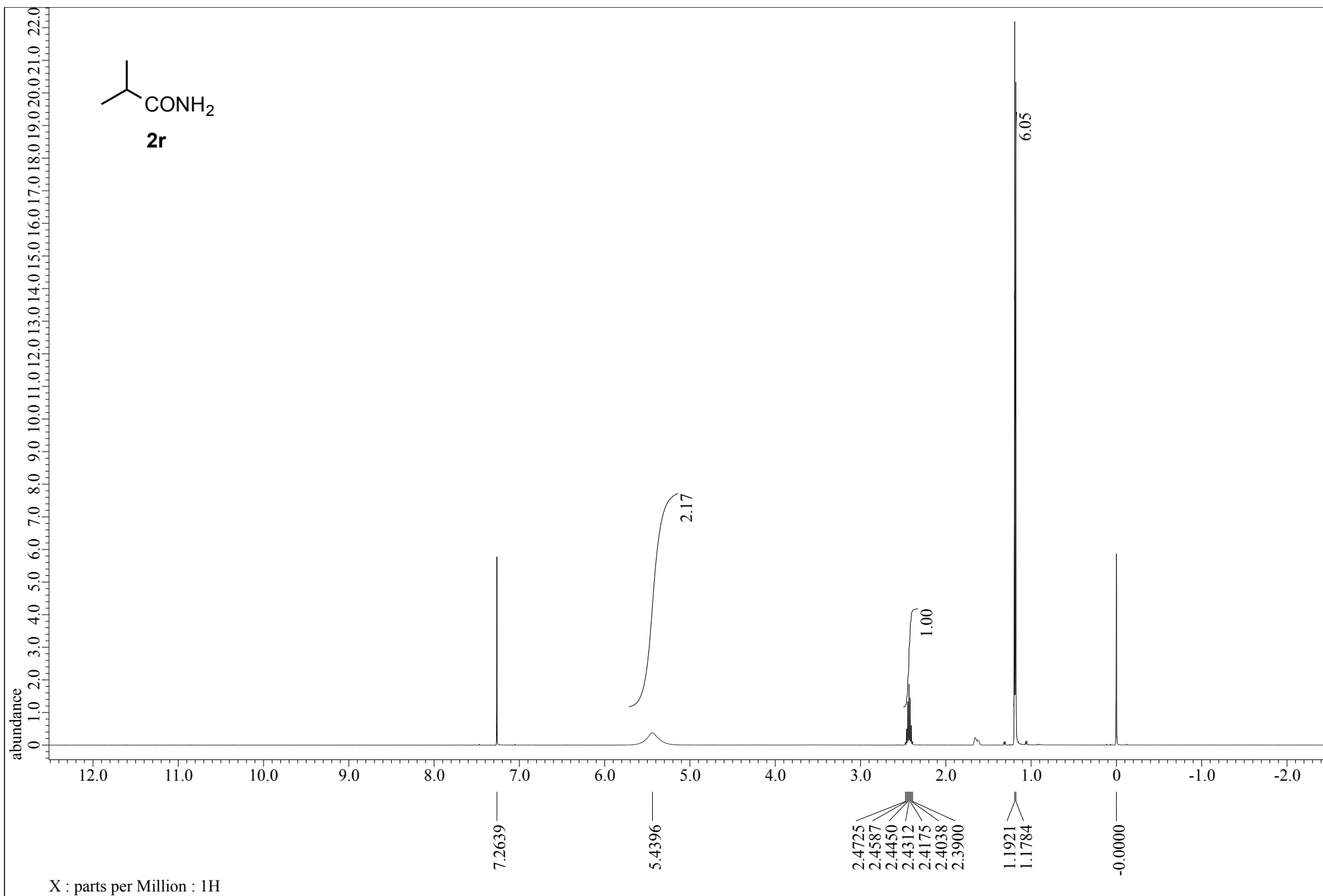
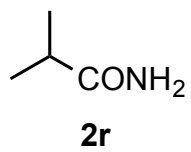
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Data_format   = 1D REAL
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Dim_units     = [ppm]
Dimensions    = X
Site          = ECA 500
Spectrometer  = JNM-ECA500

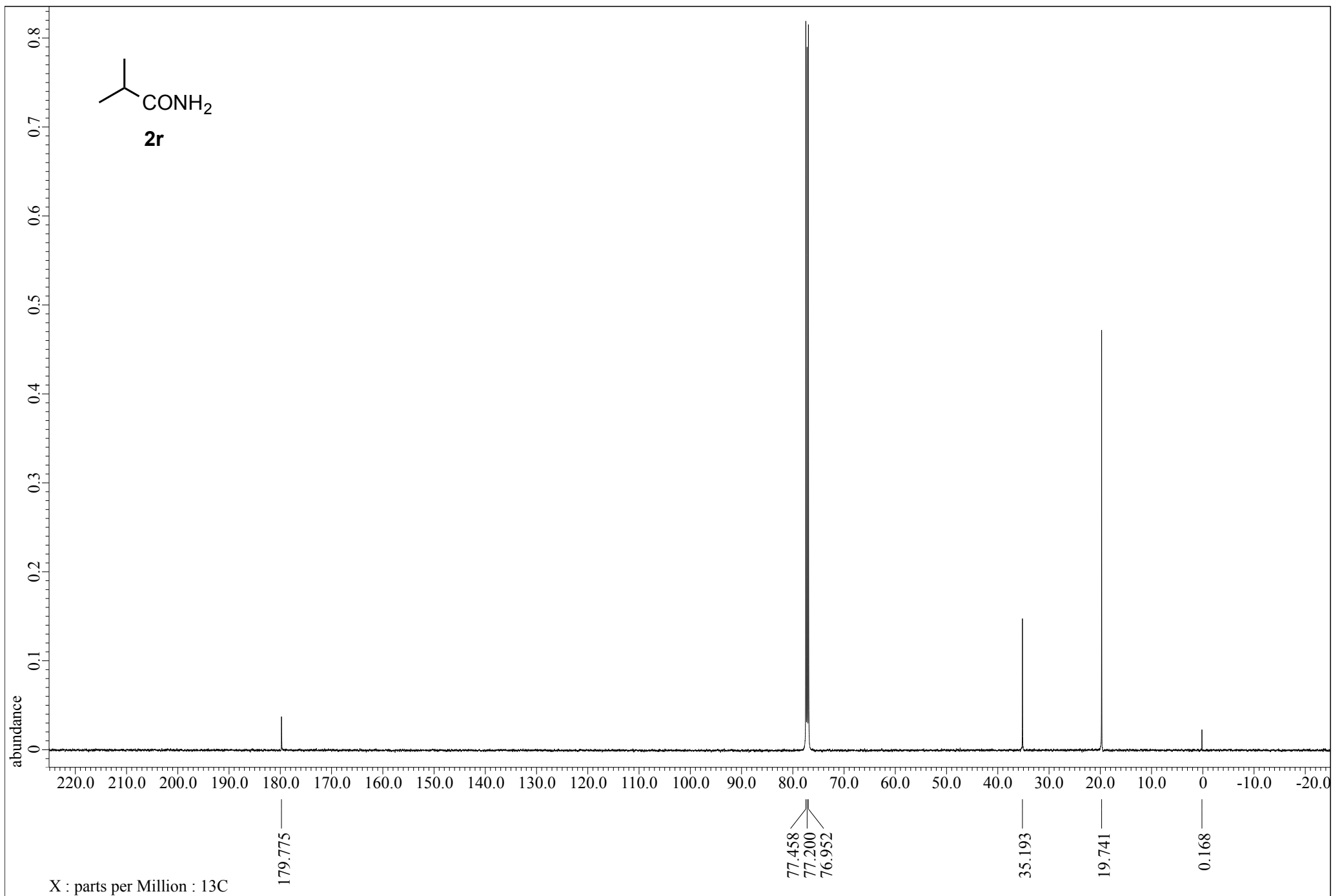
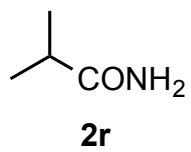
Field_strength = 11.7473579 [T] (500 [MH
X_acq_duration = 0.83361792 [s]
X_domain       = 13C
X_freq         = 125.76529768 [MHz]
X_offset       = 100 [ppm]
X_points       = 32768
X_prescans     = 4
X_resolution   = 1.19959034 [Hz]
X_sweep        = 39.3081761 [kHz]
Irr_domain     = 1H
Irr_freq       = 500.15991521 [MHz]
Irr_offset     = 5.0 [ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 12061
Total_scans    = 12061

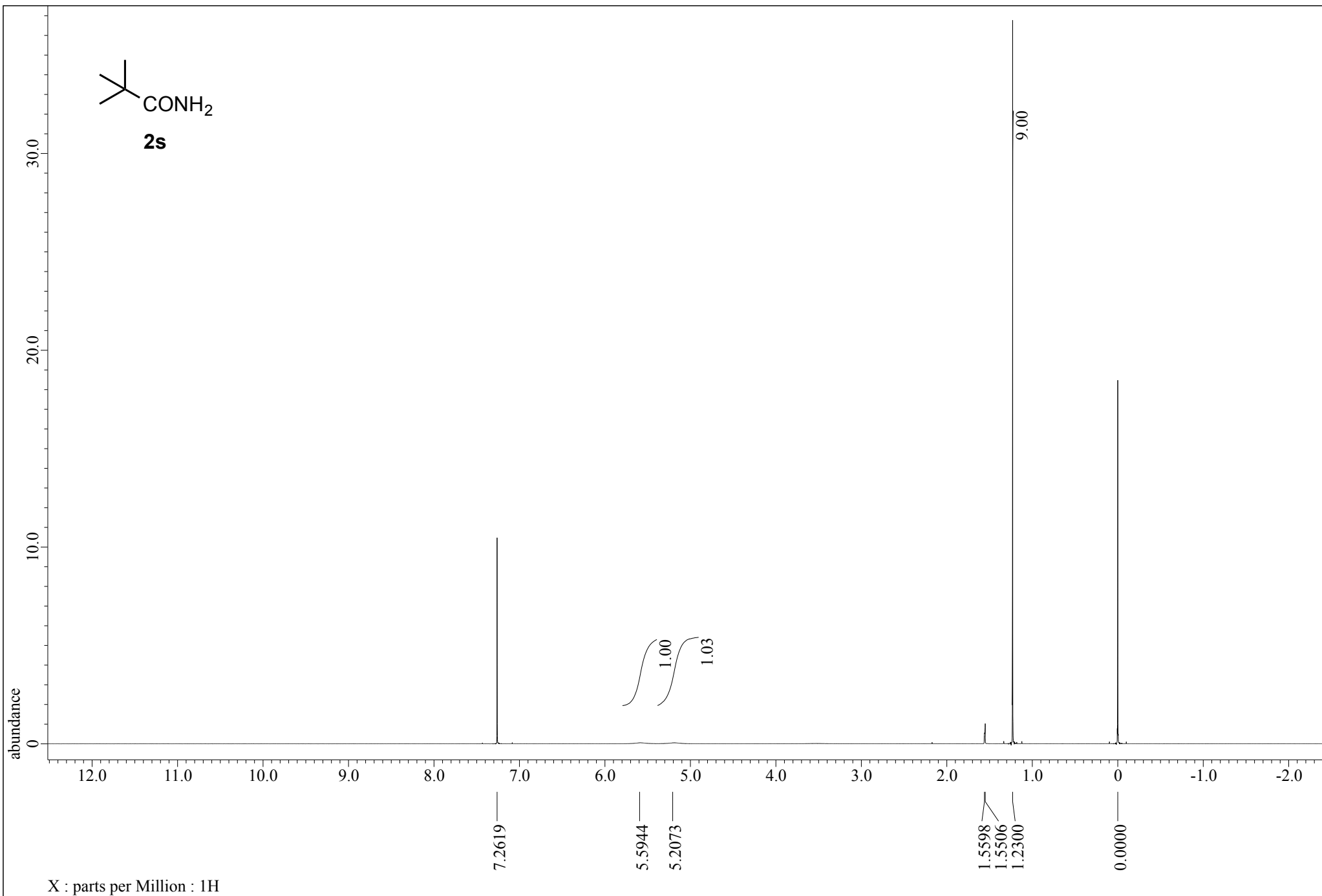
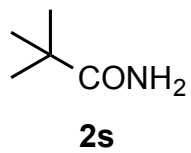
X_90_width     = 12 [us]
X_acq_time     = 0.83361792 [s]
X_angle        = 30 [deg]
X_atn          = 8.2 [dB]
X_pulse        = 4 [us]
Irr_atn_dec    = 21.707 [dB]
Irr_atn_noe    = 21.707 [dB]
Irr_noise      = WALTZ
Decoupling     = TRUE
Initial_wait   = 1 [s]
Noe            = TRUE
Noe_time       = 2 [s]
Recvr_gain     = 60
Relaxation_delay = 2 [s]
Repetition_time = 2.83361792 [s]
Temp_get       = 24.7 [dC]
  
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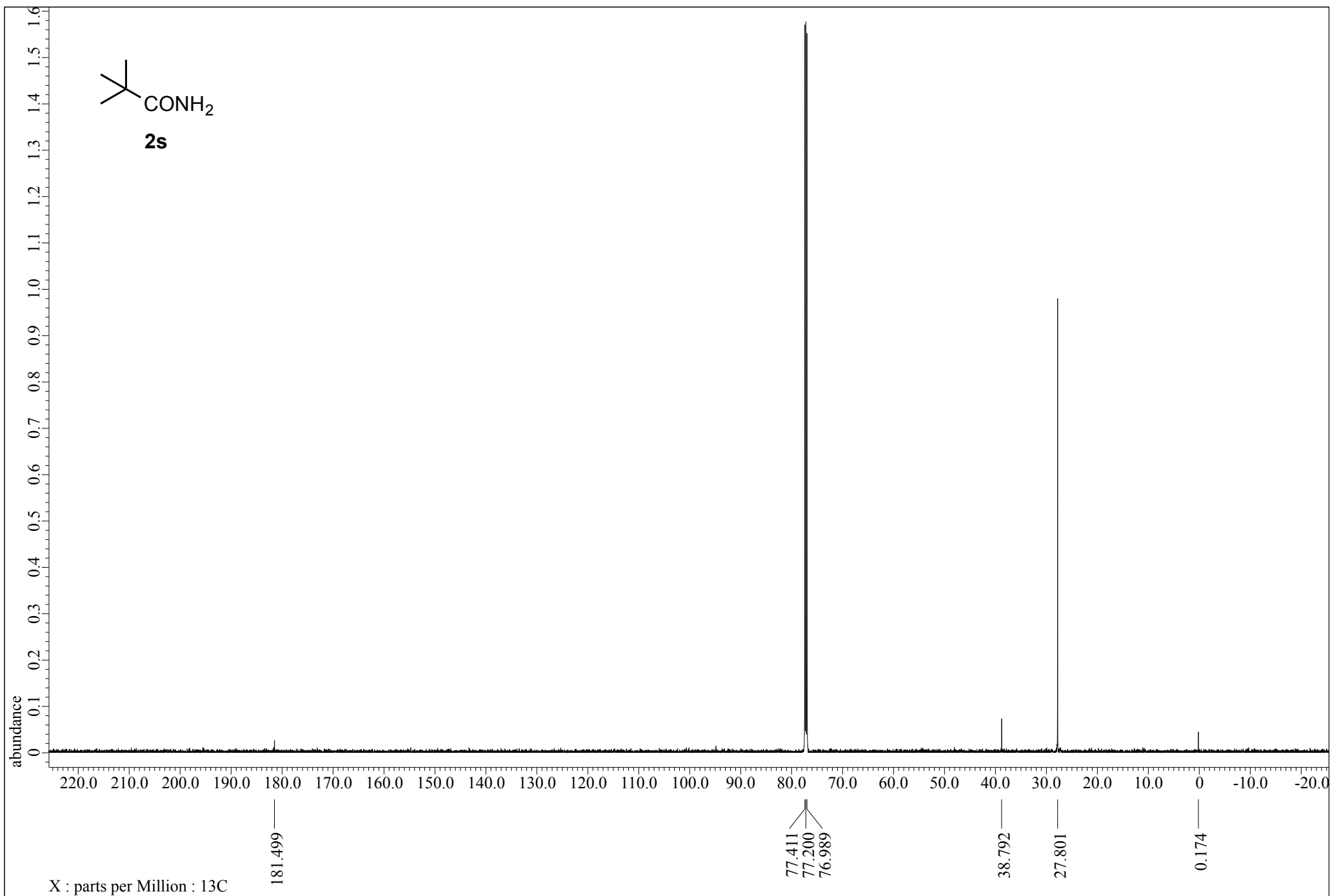
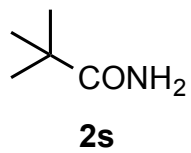


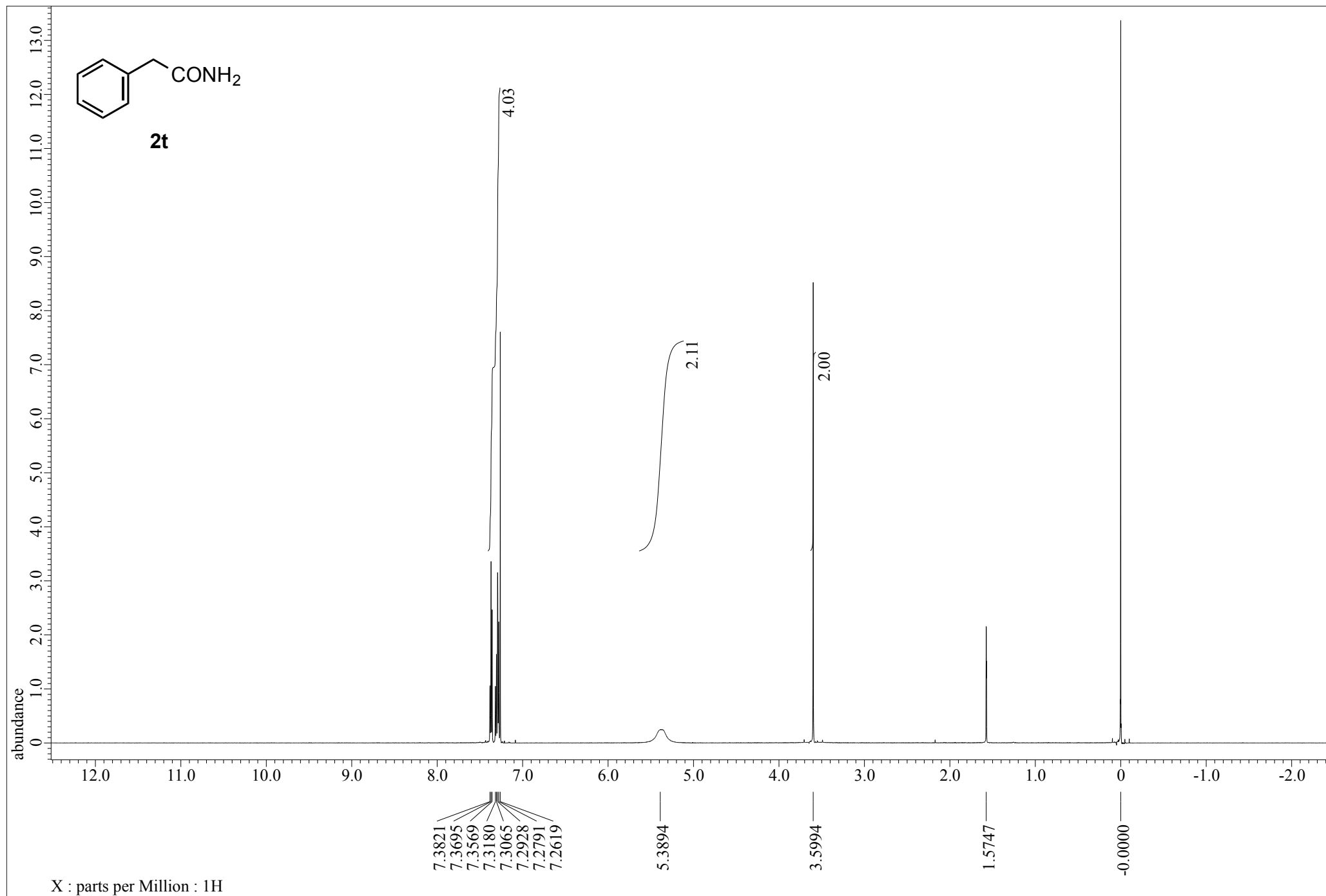


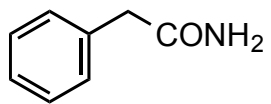




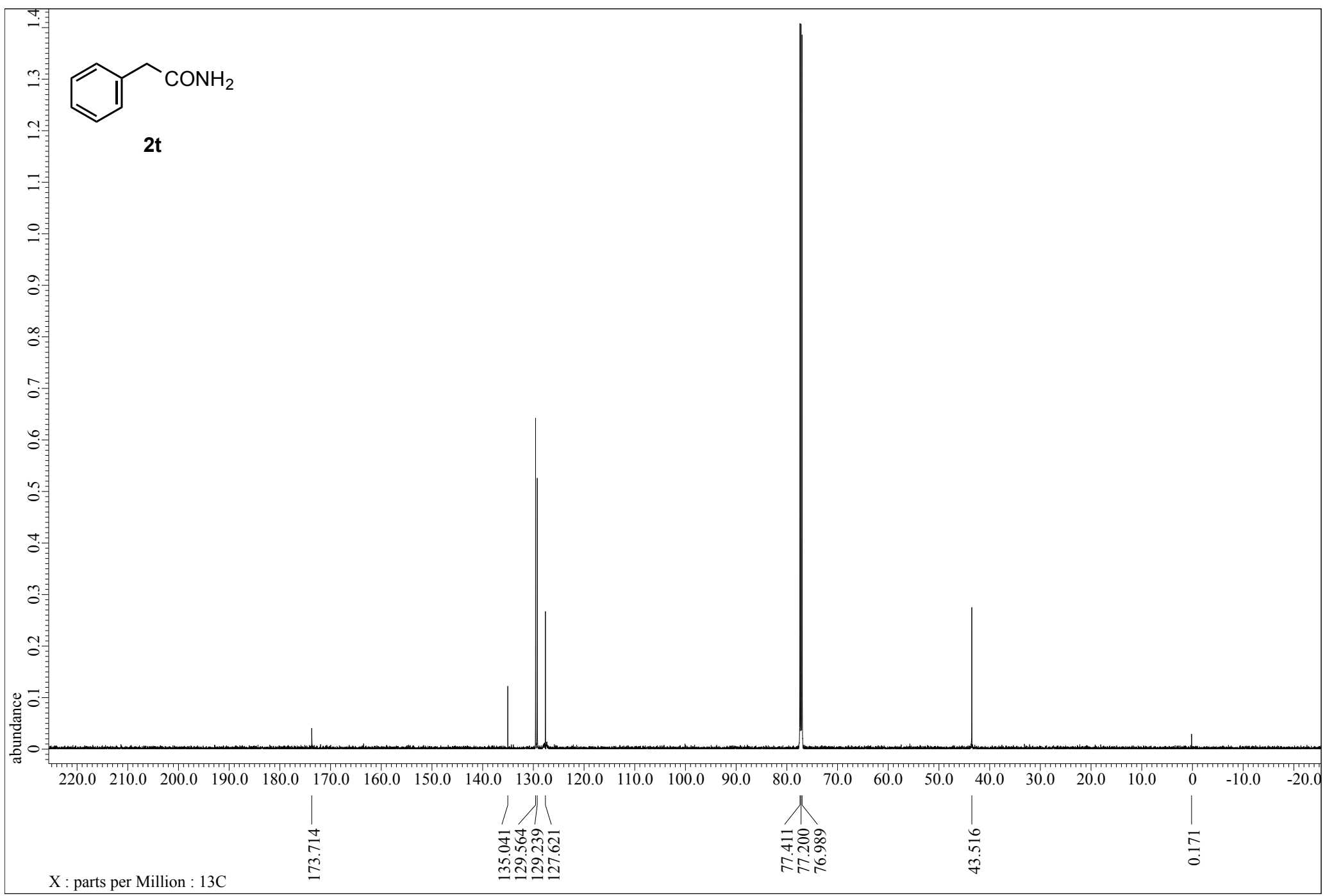


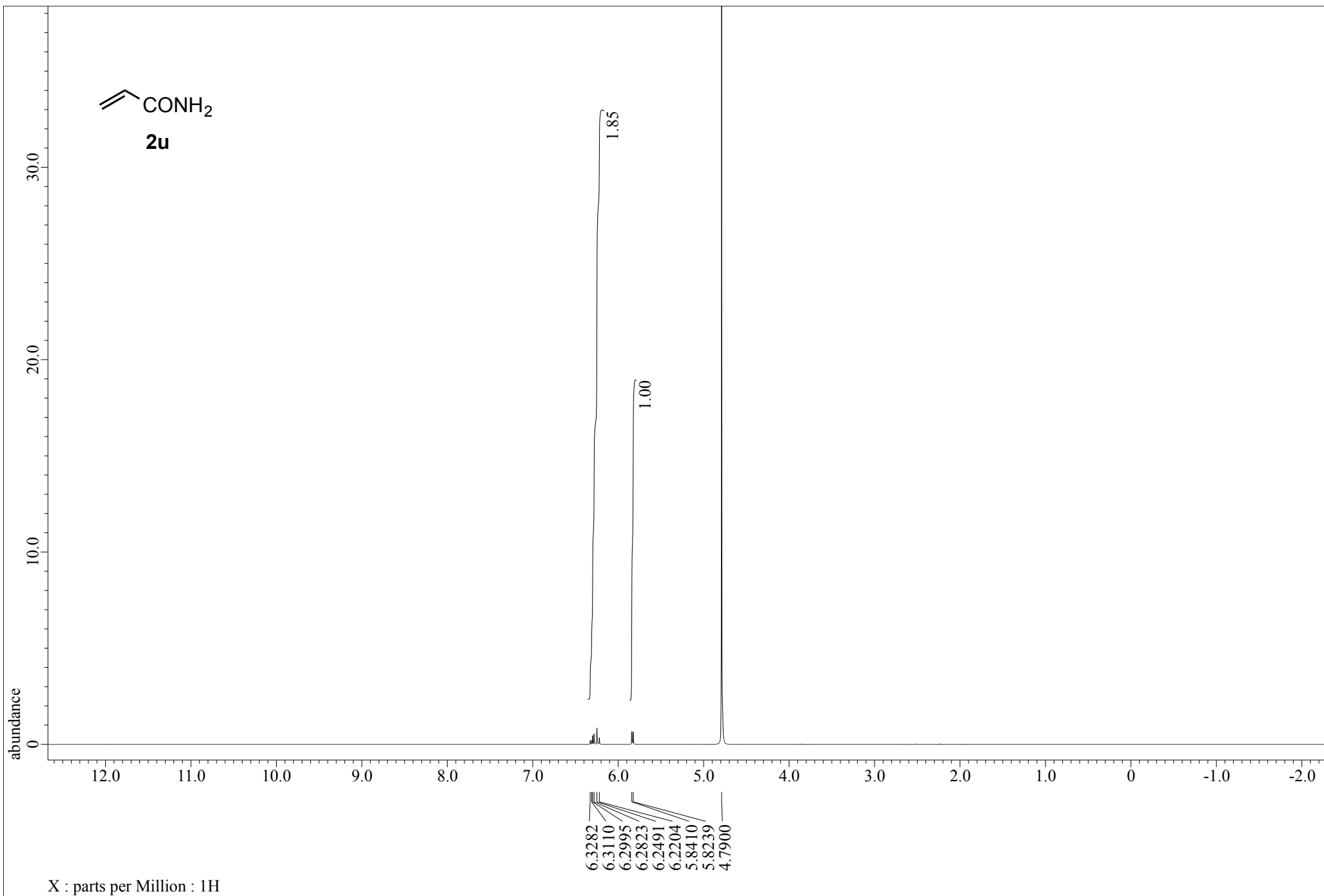
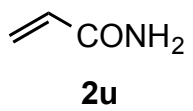


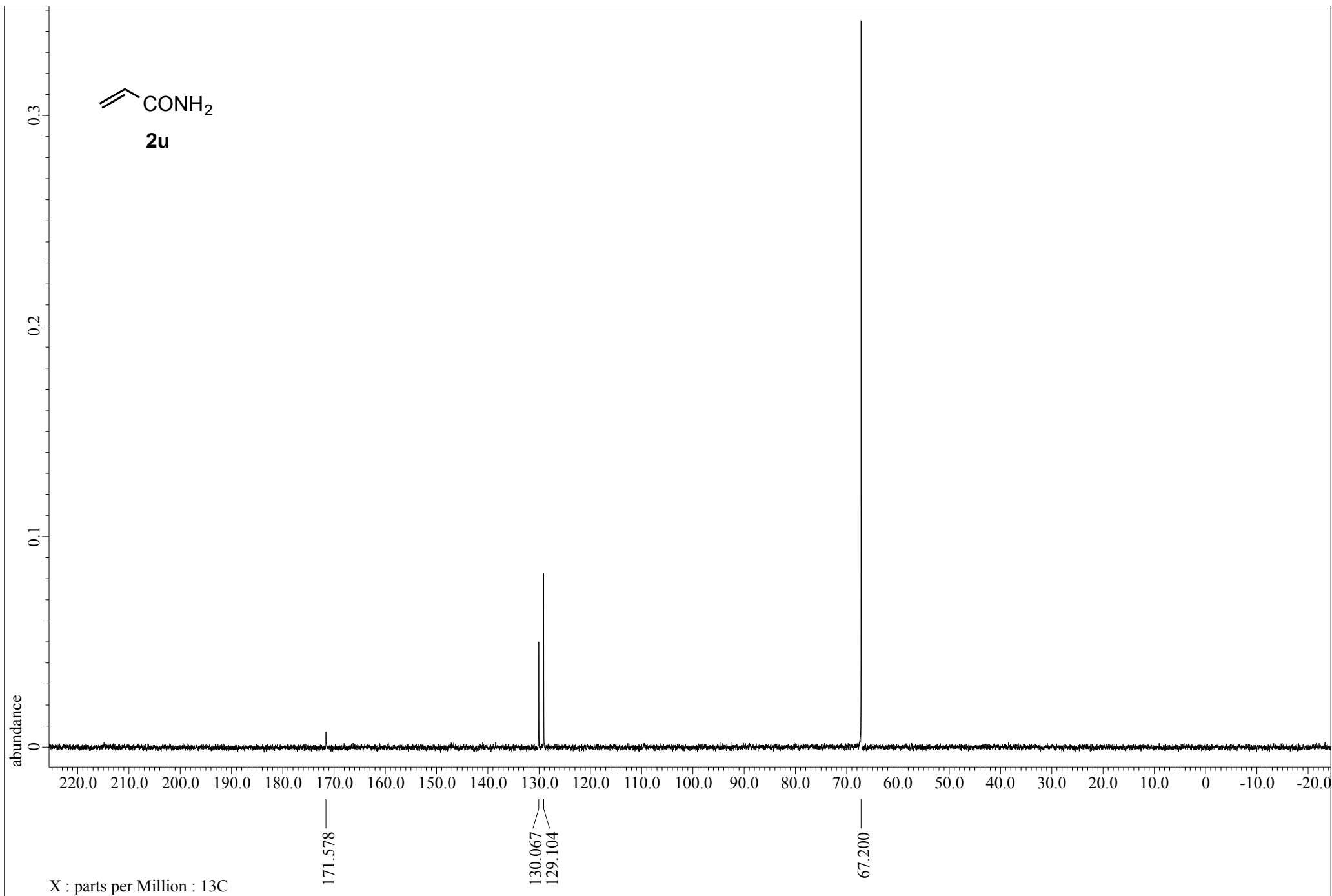
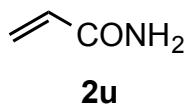


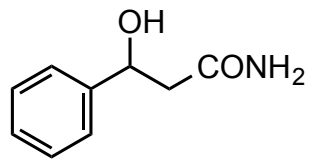


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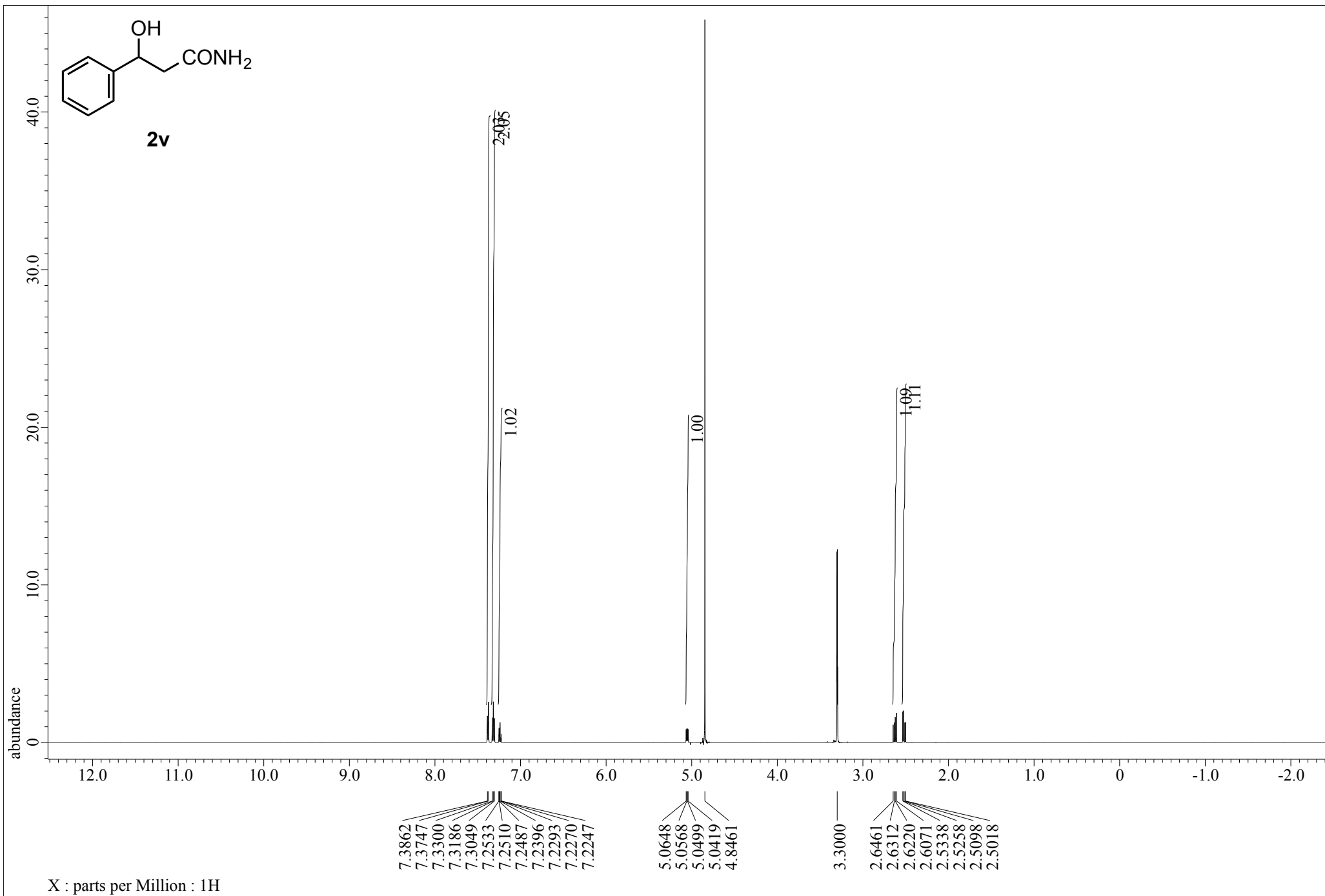


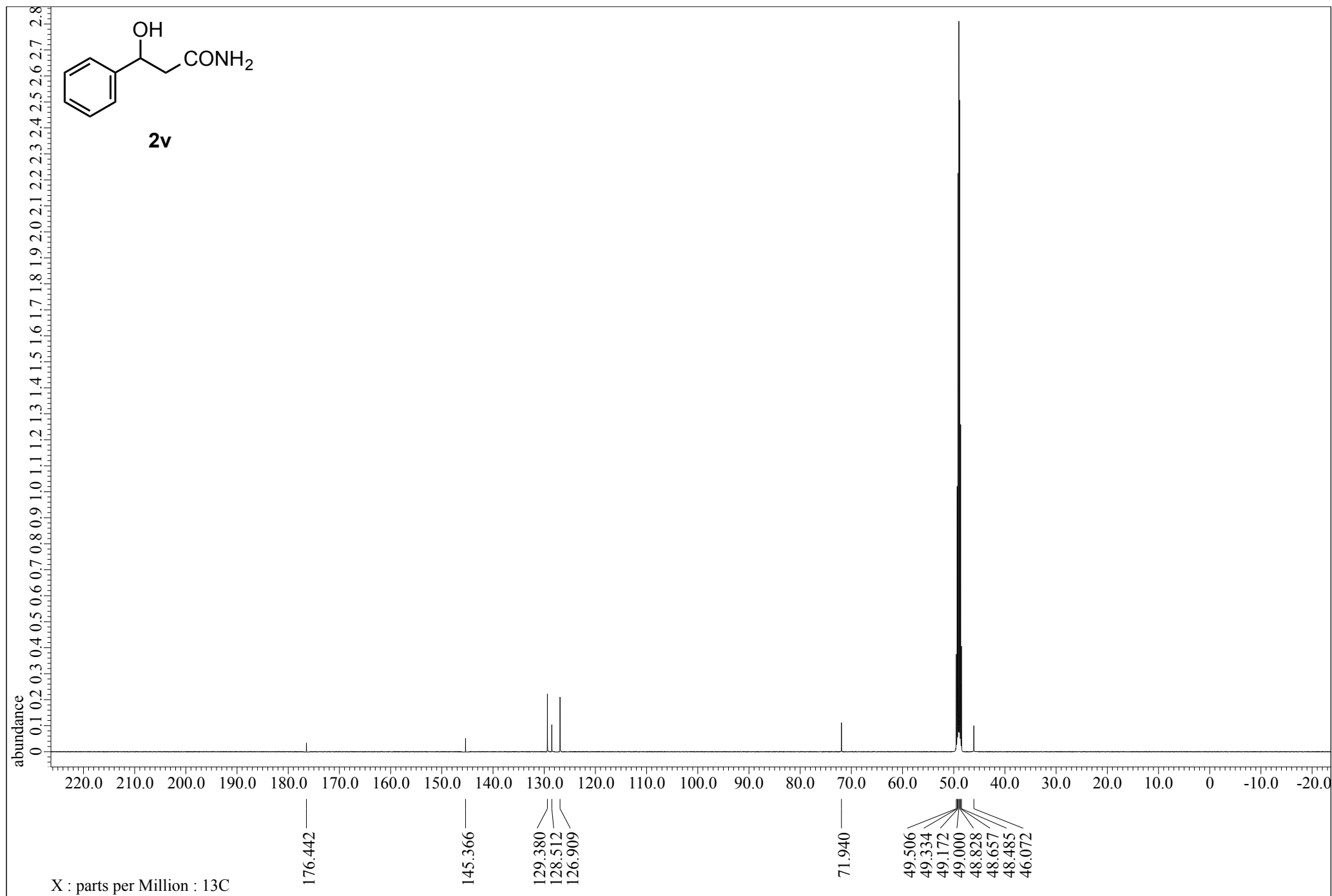


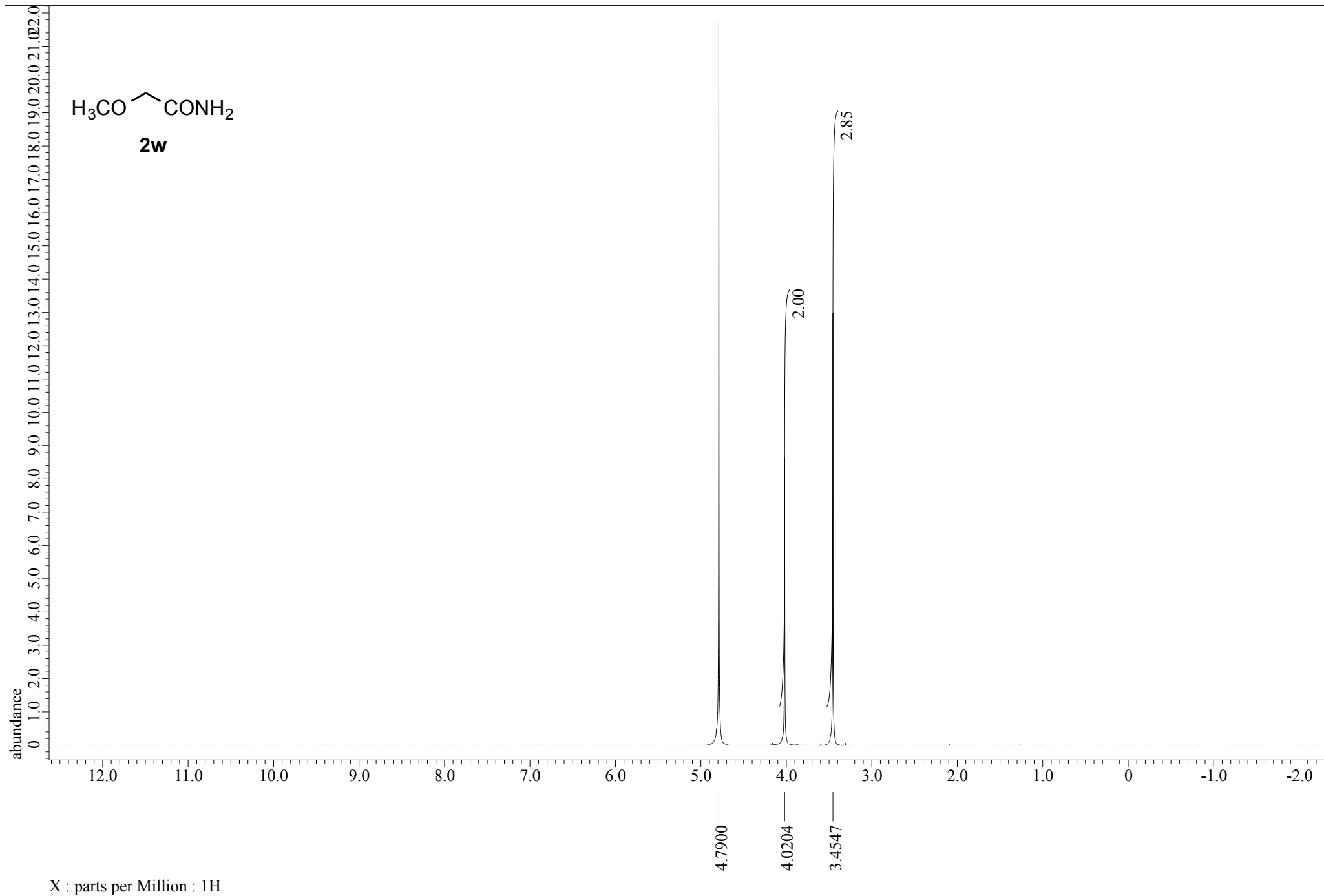


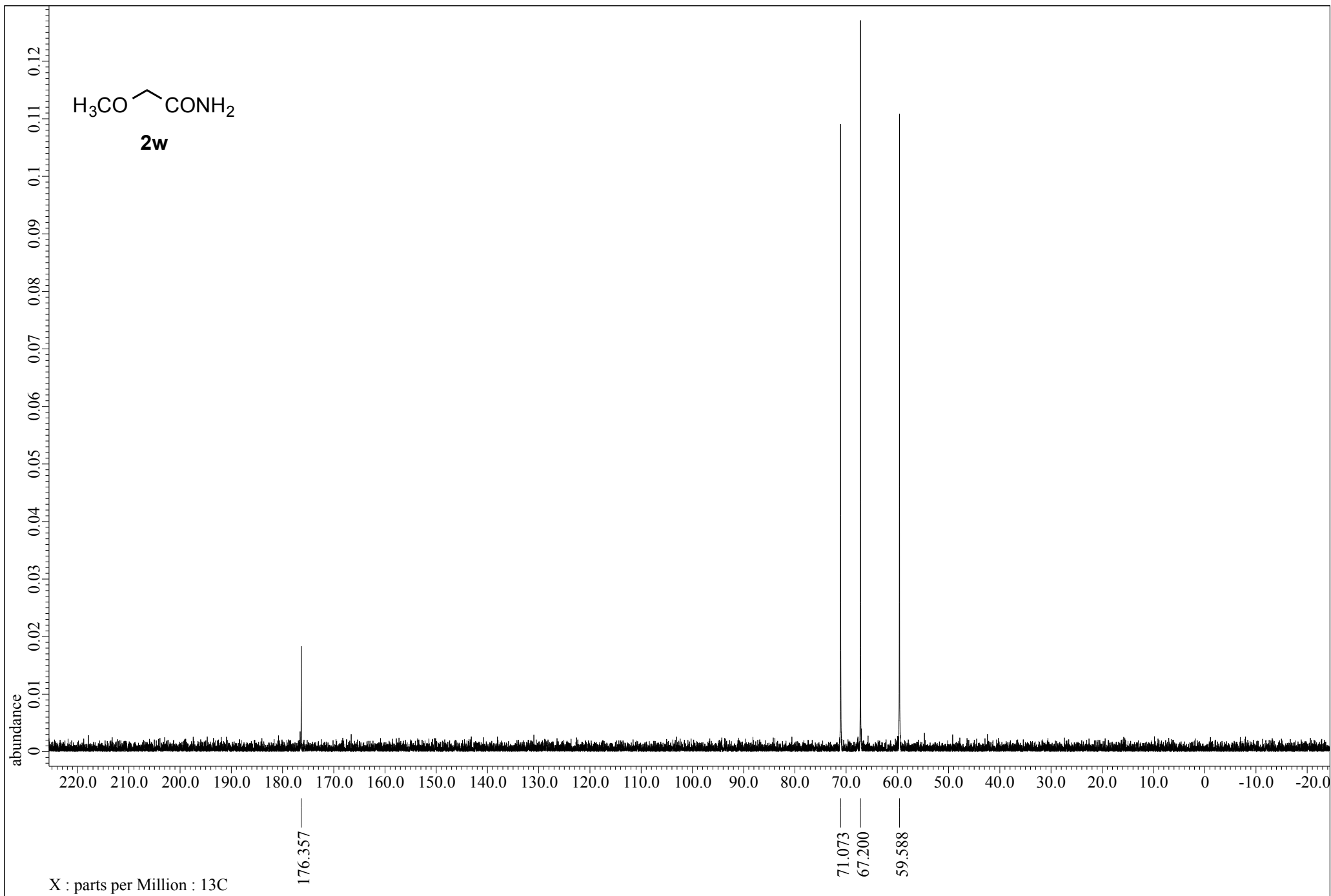
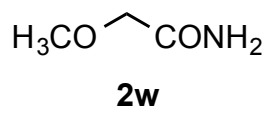


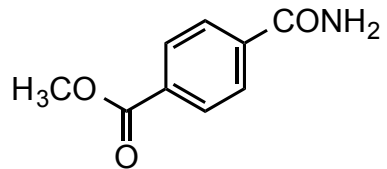
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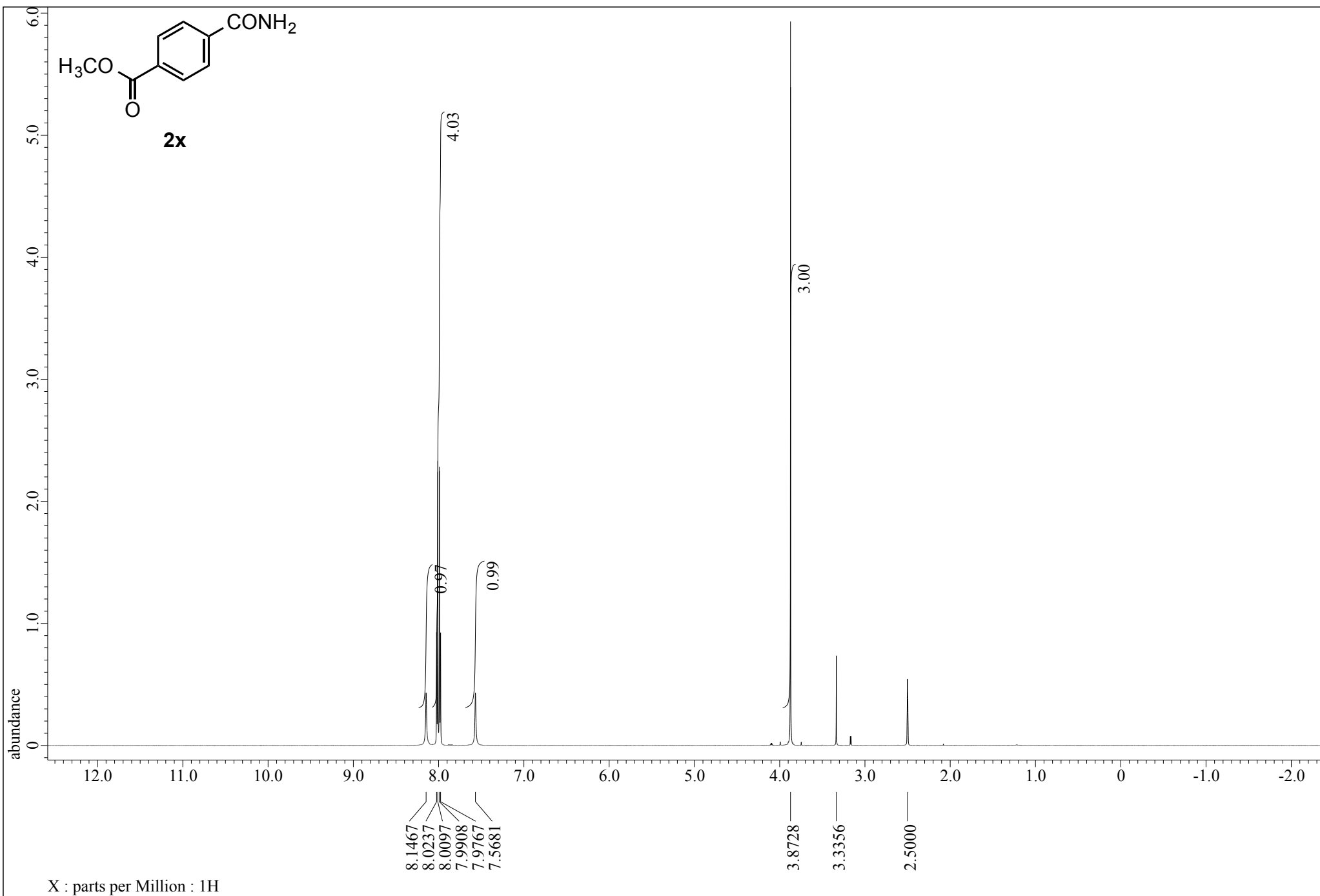


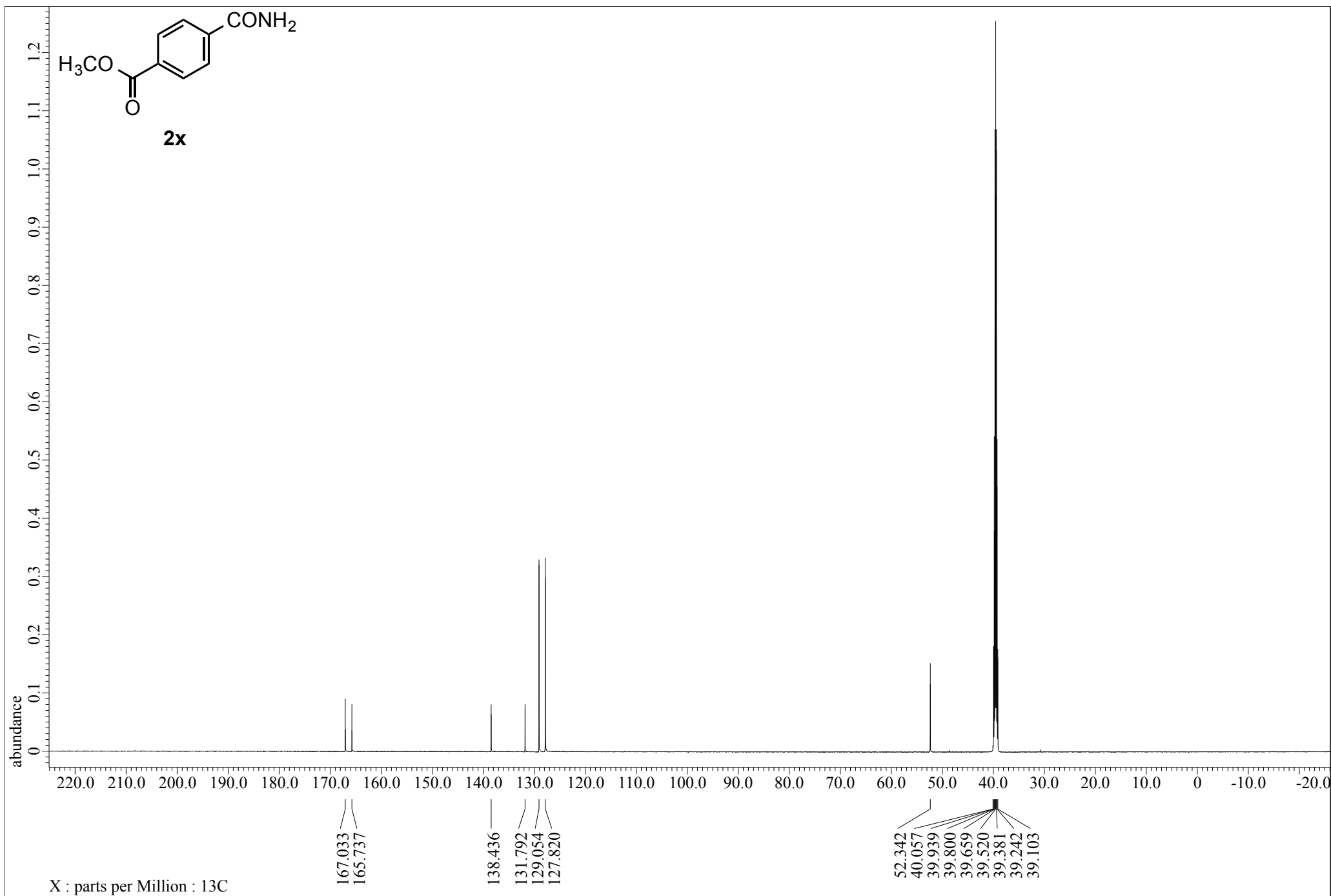


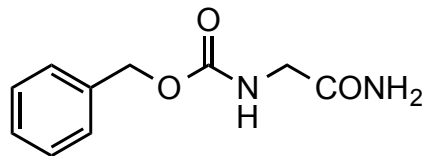




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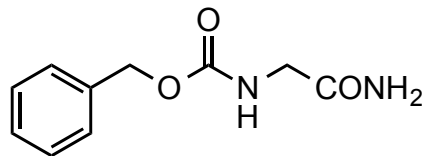
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2y

