A practical, catalytic and selective deprotection of a Boc group in *N*, *N´*-diprotected amines using iron(III)-catalysis

Juan M. López-Soria,[a] Sixto J. Pérez, [a] J. Nicolás Hernández, Miguel A. Ramírez,[a] Víctor S. Martín,[a]* and Juan I. Padrón[a,b]*

Dr. J. I. Padrón
Instituto de Productos Naturales y Agrobiología, CSIC
Francisco Sánchez, 3, 38206 La Laguna, Tenerife (Spain)
Fax: (+34)922-260-135
Juan M. López-Soria, Sixto J. Pérez, Prof. Dr. Miguel A. Ramírez, Prof. Dr. V. S. Martín, Dr. J. I. Padrón
Instituto Universitario de Bio-Orgánica "Antonio González"
Universidad de La Laguna
Francisco Sánchez, 2,38206 La Laguna, Tenerife (Spain)
jipadron@ipna.csic.es

Supporting Information

Material and Methods*:*

NMR spectra were recorded on a Bruker Avance instrument. ^{1}H NMR spectra were recorded at 400 and 500 MHz, and ^{13}C NMR were recorded at 100 and 125 MHz, VTU 298.0 °K. Chemical shifts were reported in parts per million. The residual solvent peak was used as an internal reference ($CDCl_3$: δ_H 7.26, δ_C 77.0).

Optical rotations were measured on a Perkin-Elmer 241 Polarimeter by using a Na lamp. HRESMS data were performed on a Micromass Autospec spectrometer.

For analytical thin-layer chromatography, silica gel ready-foils was used, respectively, being developed with 254 nm UV light and/or spraying with a solution of vanillin in EtOH:H_2SO_4:AcOH (15:1:1.3) and heating at 200 °C. Column chromatography was performed using silica gel (0.015-0.04 mm) and *n*-hexane/EtOAc solvent systems. All reagents were obtained from commercial sources and used without further purification. Solvents were dried and distilled before use.

Commercial Reagents

Reactive	**Company**
$FeCl_3$, 97%	Sigma-Aldrich. Made in Germany
$FeCl_3$, 99.999%	Sigma-Aldrich. Made in USA
$Fe(acac)_3$, 97%	Sigma-Aldrich. Made USA
$FeBr_2$, 98%	Sigma-Aldrich. Made USA
$FeCl_2$, 98%	Sigma-Aldrich. Made USA
$Fe(OTf)_3$, 90%	Sigma-Aldrich. Made USA
$FeCl_3.{}_6H_2O$, 97%	Sigma-Aldrich. Made USA
$InCl_3$, 98%	Sigma-Aldrich. Made USA
$RuCl_3$, Ru content:45-55%	Sigma-Aldrich. Made USA
$AuCl_3$, 99.99%	Sigma-Aldrich. Made USA
$NiCl_2$, 98%	Sigma-Aldrich. Made United Kingdom
$MnBr_2$, 98%	Sigma-Aldrich. Made USA
$CuCl_2$, 99.999%	Sigma-Aldrich. Made USA
CuCl, 99.999%	Sigma-Aldrich. Made USA
$ZnCl_2$, 99.999%	Sigma-Aldrich. Made USA
$MoCl_3$, 99.95%	Sigma-Aldrich. Made USA
$MgCl_2$, 98%	Sigma-Aldrich. Made India

General Procedures:

1- General procedure for a ferric chloride catalyzed deprotection of *N*-Boc: To a solution of the corresponding amine (1.0 equiv) in dry CH_2Cl_2 was added anhydrous $FeCl_3$ (0.3 or 1.0 equiv) in one portion. The reaction was stirred at room temperature until analysis via TLC showed complete formation of product. The reaction was quenched by addition of water with stirring for 60 min and extracted with CH_2Cl_2. The combined organics layers were dried over magnesium sulphate and the solvent was removed under reduced pressure. No further chromatography was necessary.

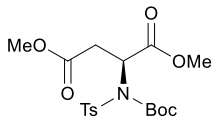
2- General procedure for ferric chloride/TMSCl catalyzed deprotection of *N*-Boc: To a solution of corresponding amine (1.0 equiv) in dry CH_2Cl_2 was added anhydrous $FeCl_3$ (0.1 equiv) and then chlorotrimethylsilane (TMSCl) (1.0 equiv). The reaction was stirred at room temperature until analysis via TLC showed complete formation of product. The reaction was quenched by addition of water with stirring for 60 min and extracted with CH_2Cl_2. The combined organics layers were dried over magnesium sulphate and the solvent was removed under reduced pressure. No further chromatography was necessary.

3- General procedure for the preparation of amino acids methyl ester hydrochlorides.
To a solution of the corresponding amino acid (1.0 equiv) in dry MeOH (0.3 M) was slowly added Me_3SiCl (4.4 equiv) at 0ºC. After the addition, the reaction was allowed to reach room temperature. The reaction was stirred at room temperature overnight, and then the solvent was removed under reduced pressure. The crude reaction was treated to the next step without further purification.

4- General procedure for tosylates, nosylates or mesylates the dimethyl ester of amino acids.
To a solution of dimethyl ester of the corresponding amino acids (1.0 equiv) in dry CH_2Cl_2 was added the corresponding sulfonyl chloride (tosyl chloride, nosyl chloride or mesyl chloride) (1.0 equiv) and then Et_3N (2.5 equiv). The reaction was stirred at room temperature until analysis via TLC showed completion of the reaction. The reaction was quenched by addition of a solution of $CuSO_4$ and extracted with CH_2Cl_2. The combined organics layers were dried over magnesium sulphate and the solvent was removed under reduced pressure. This crude reaction mixture was purified by silica gel column chromatography (*n*-hexane/EtOAc solvent systems).

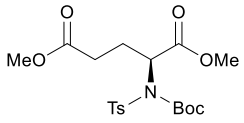
5- General procedure for *N*-Boc protection.
To a solution of the corresponding amine (1.0 equiv) in dry acetonitrile (0.7 M), Et_3N (1.5 equiv) and $(Boc)_2O$ (1.5 equiv) were sequentially added at room temperature. The reaction mixture was stirred at this temperature until analysis via TLC showed complete protection. The solvent was removed under reduced pressure and the residue triturated and washed with Et_2O using a pad of Celite. The combined organic solvents were removed under reduced pressure. This crude reaction mixture was purified by silica gel column chromatography.

Starting Materials:

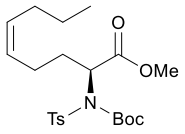


1a

Dimethyl *N*-(*tert*-butoxycarbonyl)-*N*-tosyl-*L*-aspartate (1a, Table 1): The amino acid derivative **1a** was synthesized following the general procedures described above. Spectral data was consistent with the known compound.[1]



Dimethyl *N*-(*tert*-butoxycarbonyl)-*N*-tosyl-*L*-glutamate (3, Table 2, entries 2, 9-11): This glutamate was synthesized following the general procedures described above. Spectral data was consistent with the known compound.[2]



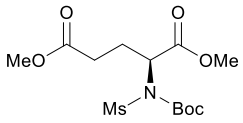
Methyl (*S*, *Z*)-2-((*N*-(*tert*-butoxycarbonyl)-4-methylphenyl)sulfonamido)non-5-enoate (3, Table 2, entries 3-5): To a solution of dimethyl *N*-(tert-butoxycarbonyl)-*N*-tosyl-L-glutamate (780 mg, 1.82 mmol) in Et_2O (0.1 M), previously cooled to -78ºC was slowly added DIBAL-H (1M, 1.82 mL). The reaction was keep at this temperature until the dimethyl ester was consumed. Then, the reaction was allowed to reach room temperature and 5.0 equiv. of H_2O per mol. of DIBAL-H were added. Once the solution becomes cloudy, Et_2O and $MgSO_4$ were added respectively. Next, the solvent of the corresponding aldehyde was filtered through a pad of celite and the solvent was removed under reduced pressure. The aldehyde crude was obtained and used without further purification.

On the other hand, a flask with a stir bar was charged with $CH_3(CH_2)_3PPh_3Br$ (945 mg, 2.36 mmol), dissolved in THF (0.1M) and cooled to 0ºC. Next, *n*-BuLi (2.5 M, 0.87 mL) was slowly added leading a change of the suspension color. After 30 min., the suspension was decanted and the supernatant solvent used to the next Wittig reaction.

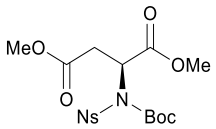
In other flask, the aldehyde crude was dissolved in THF and cooled to 0ºC. Then, we added the supernatant solvent and the reaction was allowed to reach room temperature and hydrolyzed with NH_4Cl (25 mL, saturated aqueous solution). The products were extracted with Et_2O, washed with brine, dried over anhydrous $MgSO_4$ and evaporated. This crude reaction mixture was purified by gel column chromatography (hexane: AcOEt =7:3, v:v) to obtain 600 mg (1.37 mmol) (75 % yield).

[1] J. N. Hernández, F. R. P. Crisóstomo, T. Martín, V. S. Martín, *Eur. J. Org. Chem*. 2007, 5050-5058.
[2] J. N. Hernández, M. A. Ramírez, V. S. Martín, *J. Org. Chem*, 2003, **68**, 743-746.

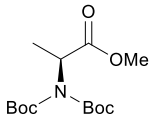
^{1}H-NMR ($CDCl_3$, 500 MHz) δ 7.93 (d, 2H), 7.31 (d, 2H), 5.44 (m, 2H), 5.08 (m, 1H), 3.72 (s, 3H), 2.44 (s, 3H), 2.26 (m, 3H), 2.04 (m, 3H), 1.37 (m, 2H), 1.28 (s, 3H), 0.9 (t, 3H) ^{13}C-NMR ($CDCl_3$, 125 MHz) δ 170.6, 150.0, 144.3, 136.8, 131.2, 129.0, 128.7, 128.0, 84.8, 59.1, 52.4, 30.6, 29.3, 28.3, 27.8, 24.4, 22.8, 21.6, 13.8. $[\alpha]_D$= -37.0 (c = 2.78, $CHCl_3$, 25 ºC). HRMS (ESI$^+$) calculated for $C_{22}H_{33}NO_6S$ 439.1457 observed 462.1926 m/z ($[M+Na]^+$).



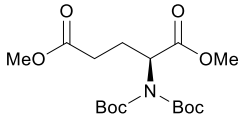
Dimethyl *N*-(*tert*-butoxycarbonyl)-*N*-(methylsulfonyl)-*L*-glutamate (**3, Table 2, entries 6-8**): ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 4.91 (m, 1H), 3.78 (s, 3H), 3.68 (s, 3H), 3.35 (s, 3H), 2.57-2.45 (m, 3H), 2.34-2.25 (m, 1H), 1.50 (s, 9H). ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 173.9, 171.2, 151.8, 86.5, 59.9, 53.7, 52.7, 42.2, 31.4, 28.9, 26.4. $[\alpha]_D$= -51.5 (c = 2.18, $CHCl_3$, 25 ºC). HRMS (ESI$^+$) calculated for $C_{13}H_{23}NO_8S$ 353.1144, observed 294.1011 m/z ($[M-COOMe]^+$).



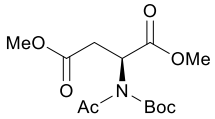
Dimethyl *N*-(*tert*-butoxycarbonyl)-*N*-(2-nitrobenzenesulfonyl)-*L*-aspartate (**3, Table 2, entries 12-14**):): ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 8.48 (m, 1H), 7.78 (m, 3H), 5.57 (m, 1H), 3.78 (s, 3H), 3.76 (s, 3H), 3.38 (m, 1H), 2.88 (dd, 1H), 1.35 (s, 9H). ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 171.4, 170.5, 150.8, 149.1, 135.2, 134.3, 133.8, 132.2, 125.6, 87.3, 56.6, 54.0, 53.1, 37.6, 28.7. $[\alpha]_D$= -2.2 (c = 3, $CHCl_3$, 25 ºC). HRMS (ESI$^+$) calculated for $C_{17}H_{23}N_2O_{10}S$ 446.0995, observed 447.1029 m/z ($[M+H]^+$).



Methyl *N, N*-di (*tert*-butoxycarbonyl)-*L*-alaninate (**3, Table 2, entries 15-17**): ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 4.99-4.93 (q, 1H), 3.72 (s, 3H), 1.50 (m, 21H). ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 172.6, 152.8, 84.1, 54.9, 53.1, 29.0, 16.6. $[\alpha]_D$= -35.3 (c = 3.17, $CHCl_3$, 25 ºC). HRMS (ESI$^+$) calculated for $C_{14}H_{25}NO_6$ 303.1682, observed 244.1549 m/z ($[M-COOMe]^+$).

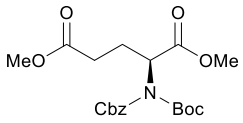


Dimethyl *N,N* di-(*tert*-butoxycarbonyl)-*L*-glutamate (**3, Table 2, entries 18-20**): This aspartate was synthesized following the general procedures described above. Spectral data was consistent with the known compound.[2]

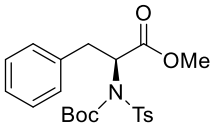


Dimethyl *N*-acetyl-*N*-(*tert*-butoxycarbonyl)-*L*-aspartate (**3, Table 2, entries 21-23**):

^{1}H-NMR ($CDCl_3$, 400 MHz) δ 5.73 (t, 1H), 3.71 (s, 3H), 3.69 (s, 3H), 3.23 (dd, 1H), 2.66 (dd, 1H), 2.50 (s, 3H), 151 (s, 9H) ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 173.4, 171.9, 171.1, 152.9, 85.5, 53.6, 53.5, 52.9, 36.2, 28.9, 27.4. $[\alpha]_D$= -30.1 (c = 5, $CHCl_3$, 25 ºC). HRMS (ESI^+) calculated for $C_{13}H_{21}NO_7$ 303.1318, observed 244.1185 m/z ($[M\text{-}COOMe]^+$).



Dimethyl *N*-benzyloxycarbonyl-*N*-(*tert*-butoxycarbonyl)-*L*-glutamate (**3, Table 2, entries 24-26**): This glutamate was synthesized following the general procedures described in reference 2. Spectral data was consistent with the known compound.[2]

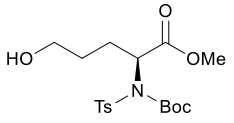


Methyl *N*-(*tert*-butoxycarbonyl)-*N*-tosyl-*L*-phenylalaninate (3, Table 2, entries 27-29): This glutamate was synthesized following the general procedures described above starting from the known precursor tosylamide.[3]

^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.33 (m, 7H), 7.14 (d, *J* = 8.0 Hz, 2H), 5.40 (dd, *J* = 5.2, 10.0 Hz, 1H), 3.51 (s, 3H), 3.60 (dd, J = 5.6, 14.4 Hz, 1H), 3.34 (dd, J= 10, 14 Hz, 1H), 2.41 (s, 3H), 1.35 (s, 9H)

^{13}C-NMR ($CDCl_3$, 100 MHz) δ 170.7, 150.6, 144.3, 137.9, 137.2, 130.2, 129.3, 129.1, 128.8, 127.2, 126.1, 85.3, 60.9, 53.0, 36.7, 28.2, 21.9

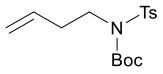
$[\alpha]_D$= -52.8 (c = 3, $CHCl_3$, 25 ºC). HRMS (ESI^+) calculated for $C_{22}H_{27}NO_6S$ 433,1559, observed 456.2028 m/z ($[M+Na]^+$).



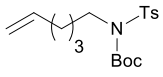
Methyl (*S*)-2-((*N*-(*tert*-butoxycarbonyl)-4-methylphenyl)sulfonamide)-5-hydroxypentanoate (3, Table 2, entries 30-32): Dimethyl *N*-(*tert*-butoxycarbonyl)-*N*-tosyl-*L*-glutamate (1g, 2.33 mmol) was added in a flask with THF (0.1 M, 23.3 mL) and the solution was cooled to -78ºC. Then, DIBAL-H was added (25.13 mmol, 5.13 mL, 1M cyclohexane) drop wise and the mixture was stirred 30 min at -78ºC. Next, the reaction was allowed to reach room temperature and 40 mL of ether and 5 eq. of water (0.46 mL) were added to the solution. Finally, an excess of $MgSO_4$ was added to this solution and the mixture was filtered through a pad of celite and the solvent evaporated. This crude reaction mixture was purified by gel column chromatography (hexane: AcOEt =5:5, v:v) to obtain 631 mg (1.57 mmol) (70 % yield).

[3] M. Ordóñez, R. De la Cruz-Cordero, M. Fernández-Zertuche, M. A. Muñoz-Hernández, O. García-Barradas, *Tetrahedron: Asymmetry* **2004**, *15*, 3035-3043.

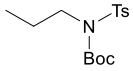
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.93 (m, 2H), 7.30 (d, J=8.4 Hz, 2H), 5.10 (m, 1H), 3.73 (m, 5H), 2.44 (s, 3H), 2.33 (m, 1H), 2.10 (m, 1H), 1.80 (m, 2H), 1.28 (s, 9H) ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 170.5, 149.9, 144.3, 136.6, 129.0, 128.6, 84.9, 62.2, 59.2, 52.4, 29.5, 27.8, 26.8, 21.6.
$[\alpha]_D$= -51.5 (c = 2.7, $CHCl_3$, 25 ºC). HRMS (ESI^+) calculated for $C_{18}H_{27}NO_7S$ 401.4740, observed 343.1450 m/z ($[M\text{-}COOMe]^+$).



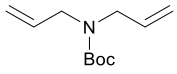
***tert*-butyl but-3-en-1-yl(tosyl)carbamate** (**Table 3, entry 1**): This carbamate was synthesized following the general procedures described above. Spectral data was consistent with the known carbamate.[4]



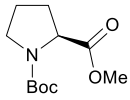
***tert*-butyl hex-5-en-1-yl(tosyl)carbamate** (**Table 3, entry 2**): This carbamate was synthesized following the general procedures describe above. Spectral data was consistent with the known carbamate.[5]



***tert*-butyl propyl(tosyl)carbamate** (**Table 3, entry 3**): This carbamate was synthesized following the general procedures described above. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.81 (d, 2H), 7.30 (d, 2H), 3.81 (t, 1H), 2.46 (s, 3H), 1.80 (q, 2H), 1.35 (s, 9H), 0.98 (t, 3H) ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 152.1, 144.9, 138.7, 130.2, 128.8, 84.9, 49.7, 28.9, 24.4, 22.6, 12.0. HRMS (ESI^+) calculated for $C_{15}H_{23}NO_4S$ 313.1348, observed 258.0800 m/z ($[M\text{-}C_4H_9\text{+}H]^+$).



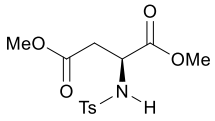
***tert*-butyl diallylcarbamate** (**Table 3, entry 4**): This carbamate was synthesized following the general procedure describe above. Spectral data was consistent with the known carbamate.[6]



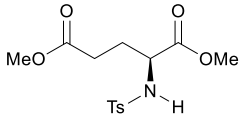
1-(*tert*-butyl) 2-methyl (*S*)-pyrrolidine-1,2-dicarboxylate (**Table 3, entry 6**): this compound was prepared from *L*-proline by the method of Confalone giving the desired methyl ester as a clear oil.[7]

[4] A. Padwa, M. Dimitroff, A. G. Waterson, T. Wu, *J. Org. Chem*. **1998**, *63*, 3986-3997.
[5] H. Ito, K. Omodera, Y. Takigawa, T. Taguchi, *Org. Lett*. **2002**, *4*, d1499-1501
[6] J. M. Muñoz-Molina, T. R. Belderrain, P. J. Pérez. *Adv. Synth. Catal*. **2008**, *350*, 2365-2372.
[7] P. Confalone, E. Huie, S. Ko. G. Cole, *J. Org. Chem*. **1988**, *53*, 482-487.

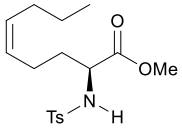
Final Materials:



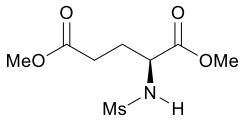
Dimethyl *N*-tosyl-*L*-aspartate (2a, Table 1): The amino acid derivatives **2a** was prepared following the general procedures of deprotection describe above. Spectral data was consistent with the known compound.[1]



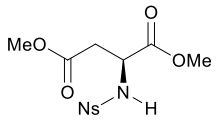
Dimethyl N-tosyl-L-glutamate (**4, Table 2, entries 2, 9-11**): This glutamate was prepared following the general procedures of deprotection describe above. Spectral data was consistent with the known compound.[2]



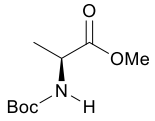
Methyl (*S, Z*)-2-((4-methylphenyl)sulfonamido)non-5-enoate (**4, Table 2, entries 3-5**): This amino acid derivative was prepared following the general procedures of deprotection describe above. ^{1}H-NMR ($CDCl_3$, 500 MHz) δ 47.71 (δ, 2H), 7.28 (d, 2H), 5.38 (m, 1H), 5.27 (m, 1H), 5.08 (d, 1H), 3.92 (m, 1H), 3.49 (s, 3H), 2.42 (s, 3H), 2.08 (m, 2H), 1.95 (m, 2H), 1.77 (m, 1H), 1.68 (m, 1H), 1.65 (m, 1H), 1.36 (m, 2H), 0.88 (t, 3H). ^{13}C-NMR ($CDCl_3$, 125 MHz) δ 172.1, 143.6, 136.8, 131.6, 129.6, 127.3, 55.5, 52.4, 33.5, 29.2, 22.8, 22.6, 21.5, 13.7. $[\alpha]_D$= +24.6 (c=2.1, $CHCl_3$, 25 ºC). HRMS (ESI^+) MS calculated for $C_{17}H_{25}NO_4S$ 339.1504, observed 340.1583 m/z ($[M+H]^+$).



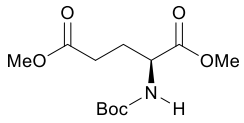
Dimethyl *N*-(methylsulfonyl)-*L*-glutamate (**4, Table 2, entries 6-8**): This aspartate was prepared following the general procedures of deprotection describe above. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 5.04 d, 1H), 3.80 (s, 3H), 3.69 (s, 3H), 2.96 (s, 3H), 2.56-2.46 (m, 2H), 2.29-2.19 (m, 1H), 1.99-196 (m, 1H). ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 174.1, 173.2, 56.3, 53.9, 52.9, 42.2, 30.7, 29.2. $[\alpha]_D$= -8.8 (c = 2.3, $CHCl_3$, 25 ºC). HRMS (ESI^+) calculated for $C_8H_{15}NO_6S$ 253.0620, observed 195.0565 m/z ($[M-COOMe]^+$).



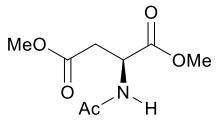
Dimethyl *N*-(2-nitrobenzenesulfonyl)-*L*-aspartate (**4, Table 2, entries 12-14**): This aspartate was prepared following the general procedures of deprotection describe above. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 8.10 (m, 1H), 7.60 (m, 1H), 7.74 (m, 2H), 6.65 (d, 1H), 4.46 (m, 1H), 3.70 (s, 3H), 3.53 (s, 3H), 3.13-3.07 (dd, 1H), 2.95-290 (dd, 1H). ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 171.7, 171.1, 148.6, 135.4, 134.6, 133.9, 131.4, 126.5, 54.0, 53.8, 53.2, 38.5. $[\alpha]_D$= -150.0 (c = 1.0, $CHCl_3$, 25 ºC). HRMS (ESI$^+$) calculated for $C_{12}H_{14}N_2O_8S$ 346.0471, observed 347.0511 m/z ($[M+H]^+$).



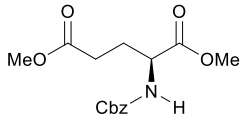
Methyl *N*-(*tert*-butoxycarbonyl)-*L*-alaninate (**3, Table 2, entries 15-17**): This alaninate was prepared following the general procedures of deprotection describe above. Spectral data was consistent with the known compound.[8]



Dimethyl *N*-(*tert*-butoxycarbonyl)-*L*-glutamate (**4, Table 2, entries 18-20**): This aspartate was synthesized following the general procedures describe above. Spectral data was consistent with the known compound.[2]

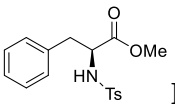


Dimethyl *N*-acetyl-*L*-aspartate (**4, Table 2, entries 21-23**): This aspartate was synthesized following the general procedures describe above. ^{1}H-NMR ($CDCl_3$, 400 MHz) δ 6.47 (m, 1H), 4.86 (m, 1H), 3.77 (s, 3H), 3.70 (s, 3H), 3.03 (dd, 1H), 2.86 (dd, 1H), 2.04 (s, 3H) ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 172.6, 172.2, 170.8, 53.8, 53.0, 49.5, 37.1, 24.1. $[\alpha]_D$= +28.5 (c = 3.0, $CHCl_3$, 25 ºC). HRMS (ESI$^+$) calculated for $C_8H_{13}NO_5$ 203.0794, observed 204.1205 m/z ($[M+H]^+$)

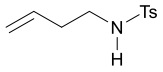


Dimethyl *N*-benzyloxycarbonyl-*L*-glutamate (**4, Table 2, entries 24-26**): This aspartate was synthesized following the general procedures describe above. Spectral data was consistent with the known compound.[2]

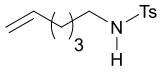
[8] M. L. Di Gioia, A. Barattuci, P. Bonaccorsi, A. Leggio, L. Minuti, E. Romio, A. Temperini, C. Siciliano, *RSC Adv.*, **2014**, *4*, 2678-2686.



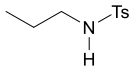
Methyl tosyl-*L*-phenylalaninate (**4, Table 2, entries 27-29**): This aspartate was synthesized following the general procedures describe above. Spectral data was consistent with the known compound.[3]



N-(but-3-en-1-yl)-4-methylbenzenesulfonamide (**Table 3, entry 1**): This sulfonamide was synthesized following the general procedures describe above. Spectral data was consistent with the known sulfonamide.[4]



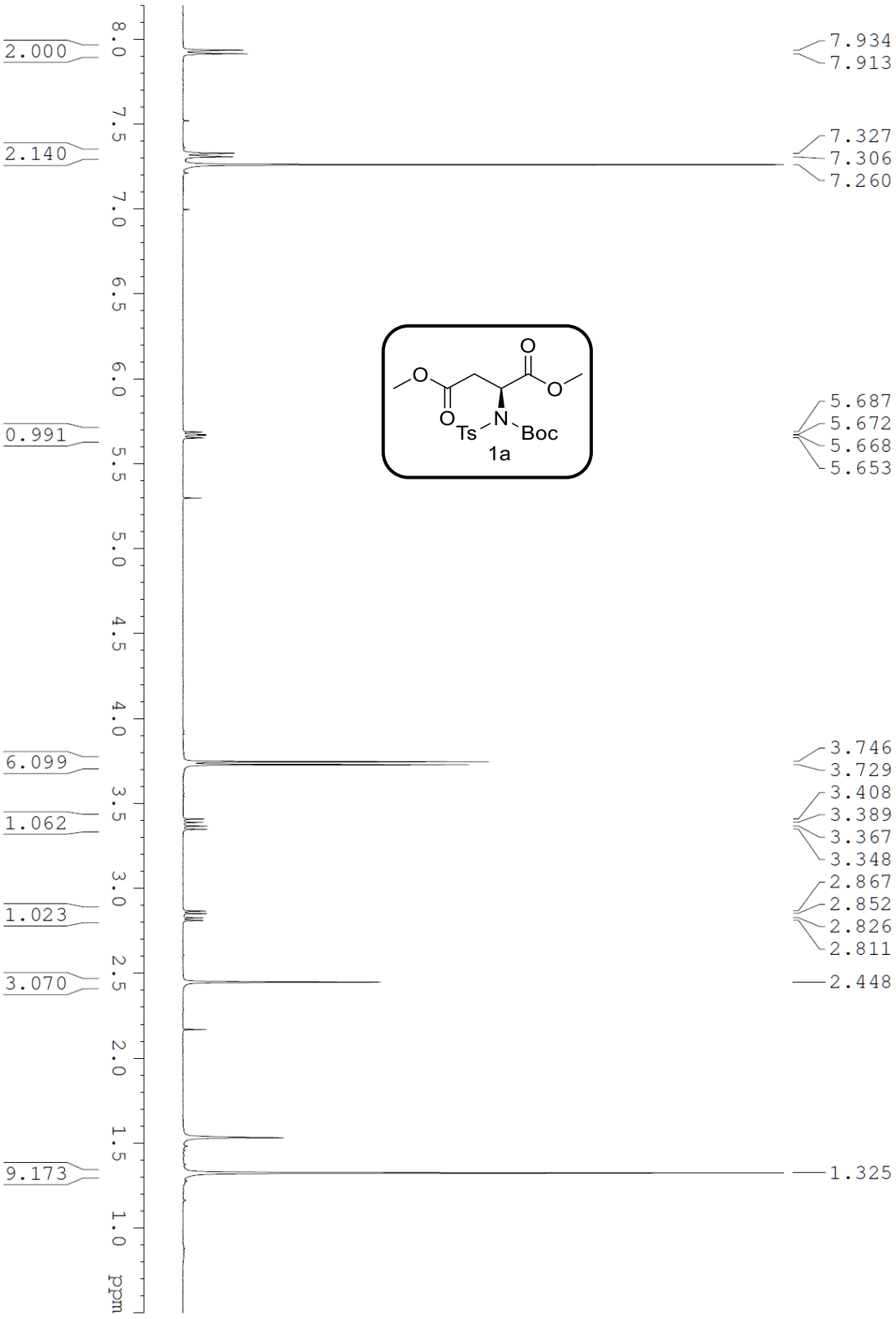
***N*-(hex-5-en-1-yl)-4-methylbenzenesulfonamide** (**Table 3, entry 2**): This sulfonamide was synthesized following the general procedures describe above. Spectral data was consistent with the known sulfonamide.[9]

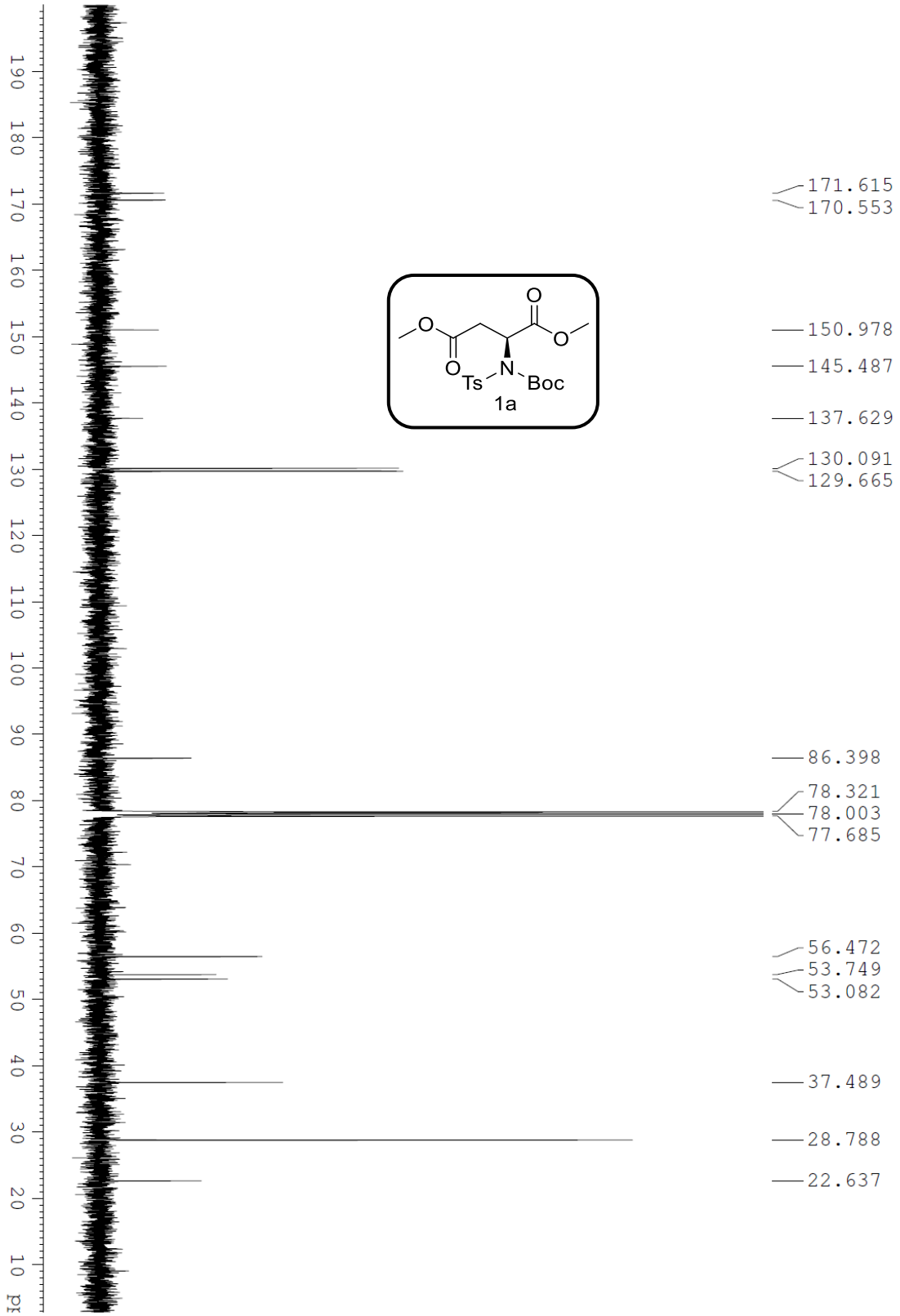


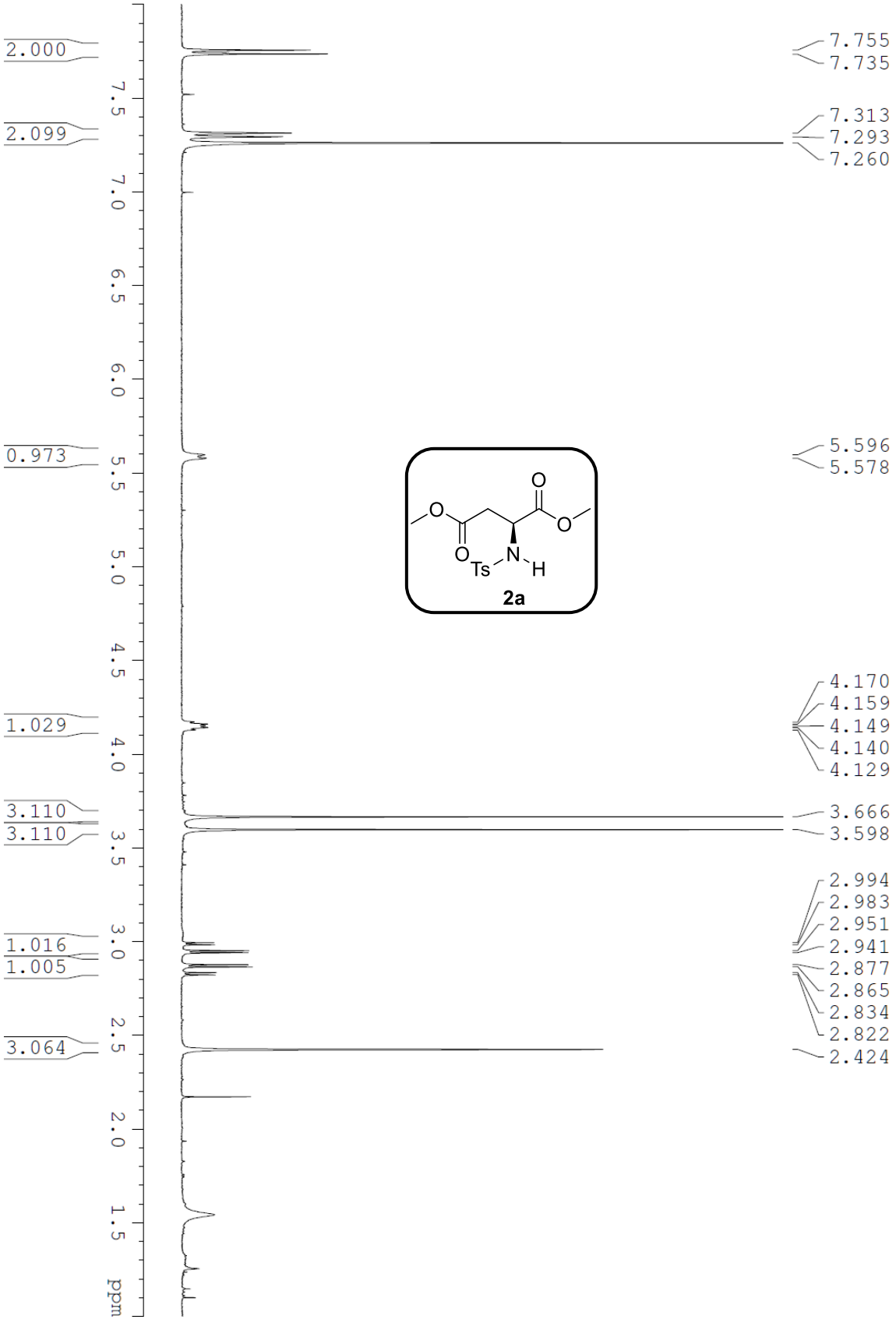
4-methyl-N-propylbenzenesulfonamide (**Table 3, entry 3**): This sulfonamide was synthesized following the general procedures describe above. Spectral data was consistent with the known sulfonamide.[10]

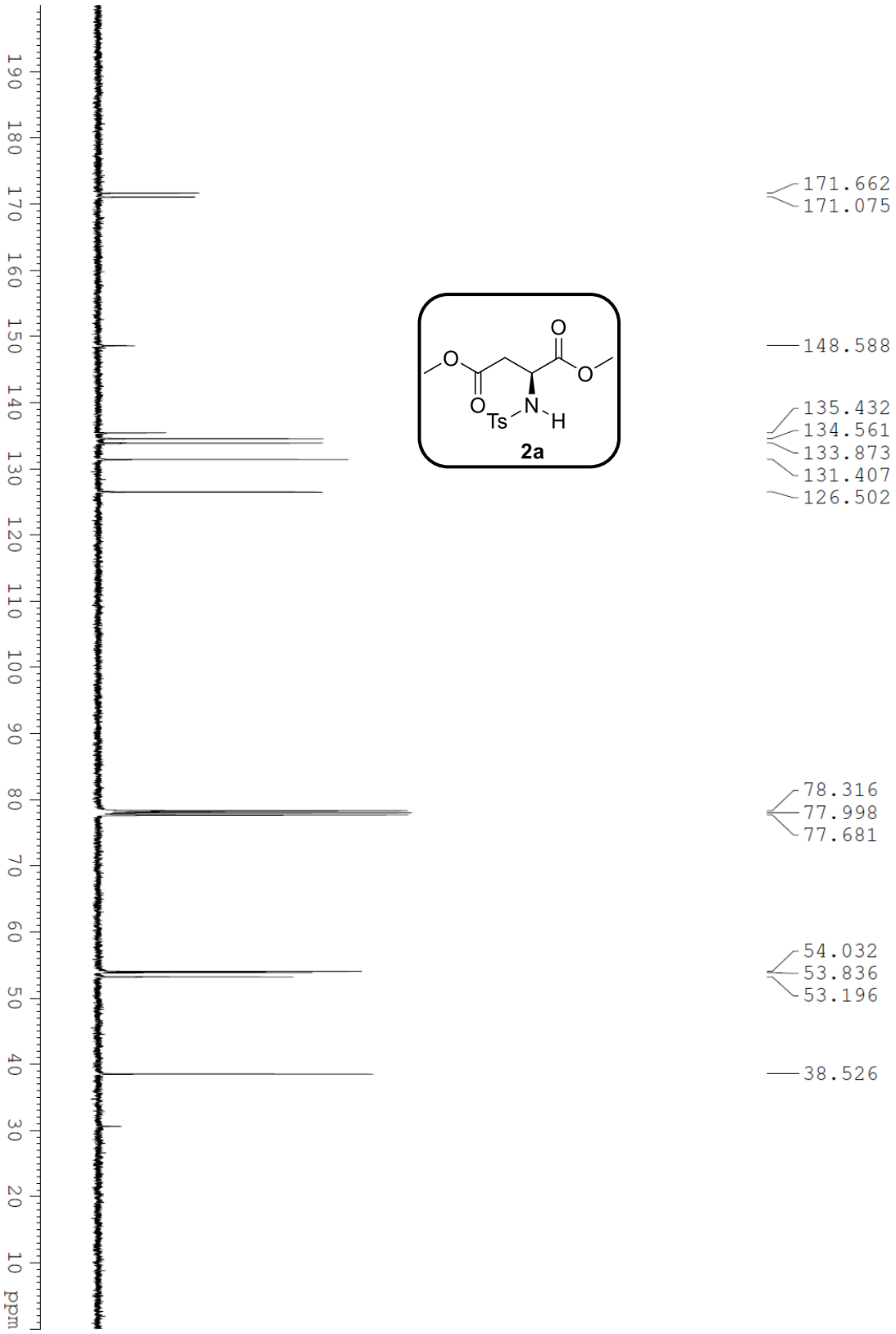
[9] T. Aubineau, J. Cossy, *ChemComm*., **2013**, *49*, 3303-3305.
[10] X. Tang, L. Huang, C. Qi, X . Wu, W. Wu, H. Jiang, *ChemComm*., **2013**, *49*, 6102-6104

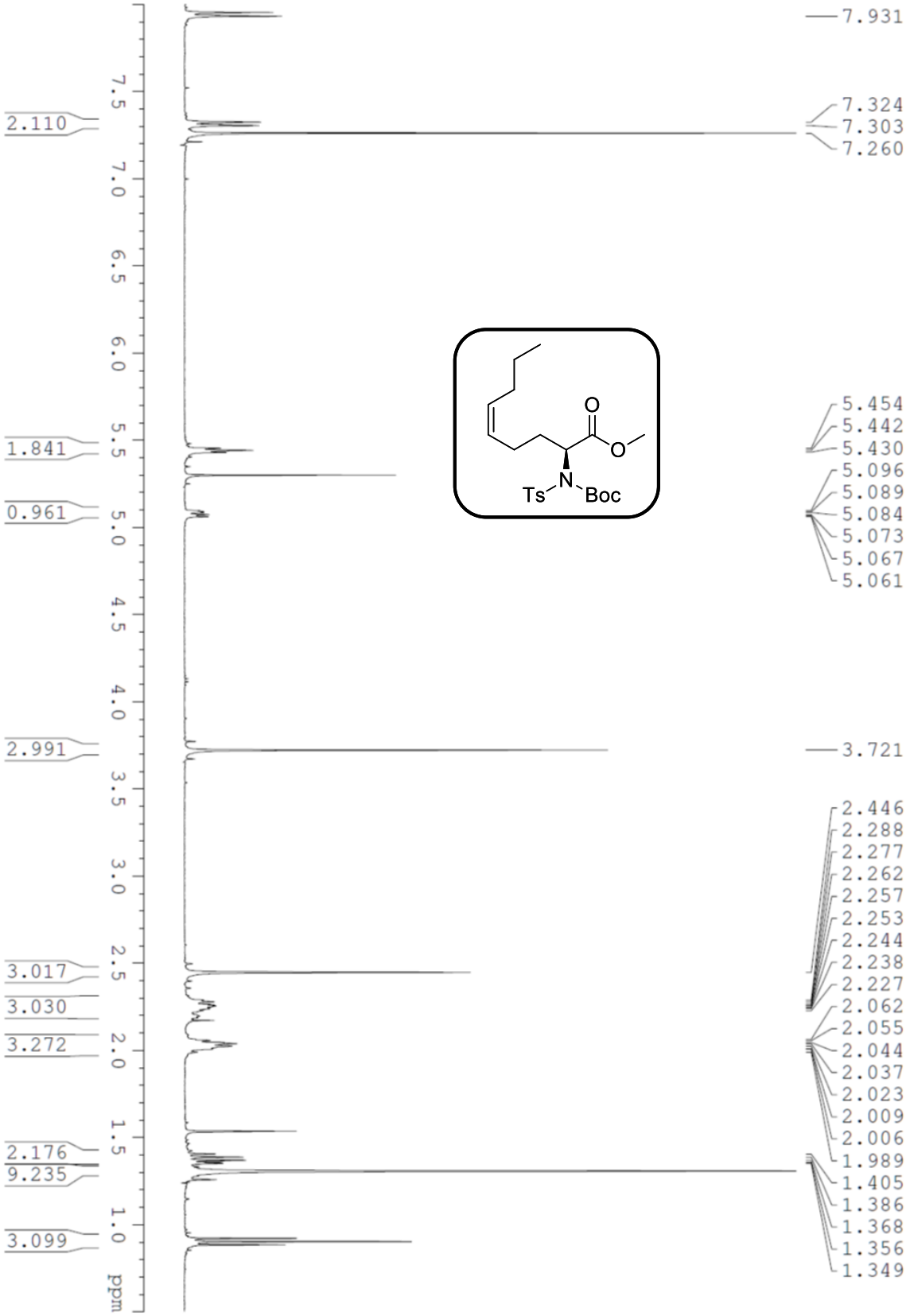
NMR section
(All these spectra are from the crude reaction)

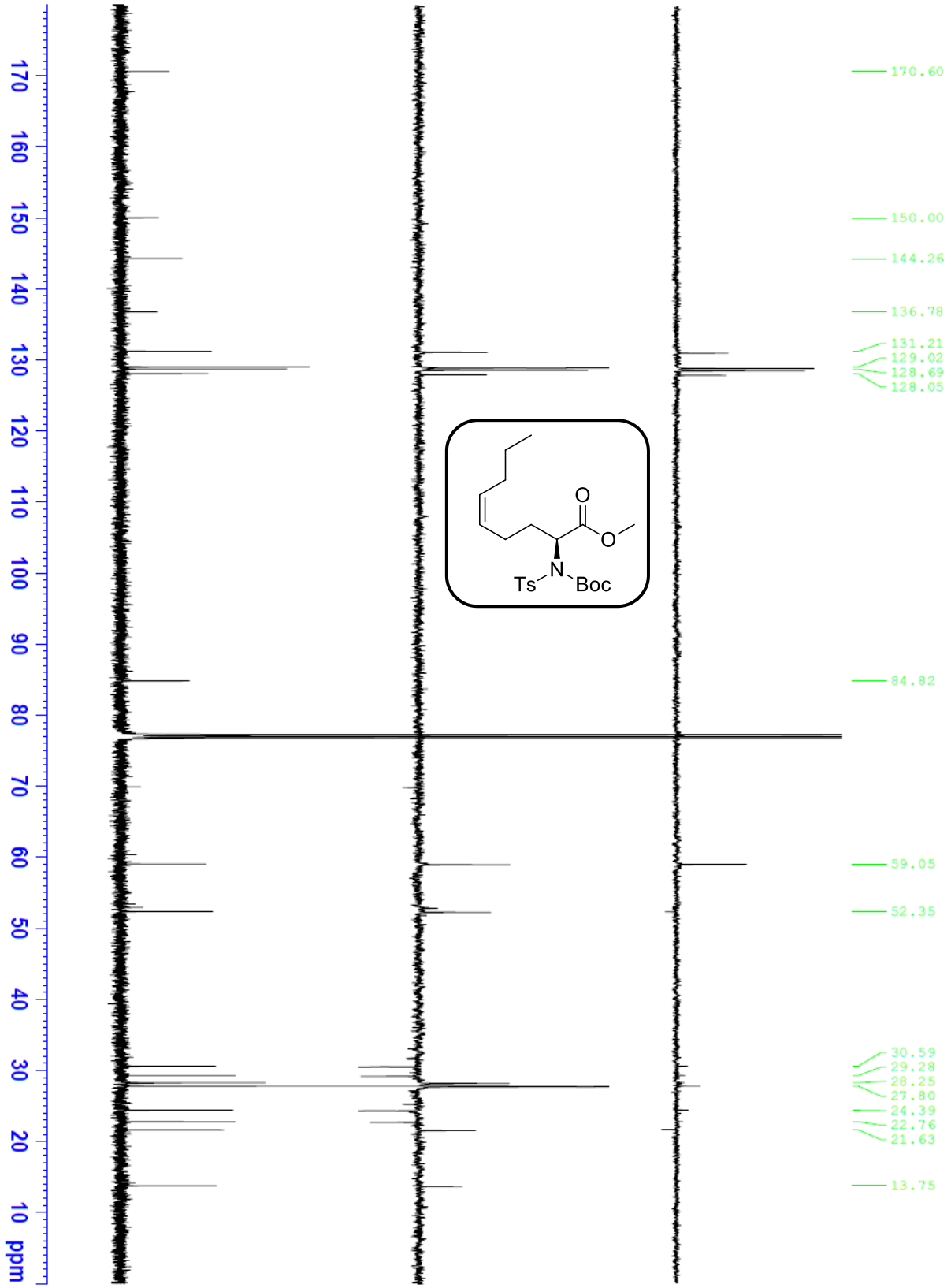

2.000
2.140
0.991
6.099
1.062
1.023
3.070
9.173
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
7.934
7.913
7.327
7.306
7.260
5.687
5.672
5.668
5.653
3.746
3.729
3.408
3.389
3.367
3.348
2.867
2.852
2.826
2.811
2.448
1.325
O
O
O
O
N
Ts
Boc
1a

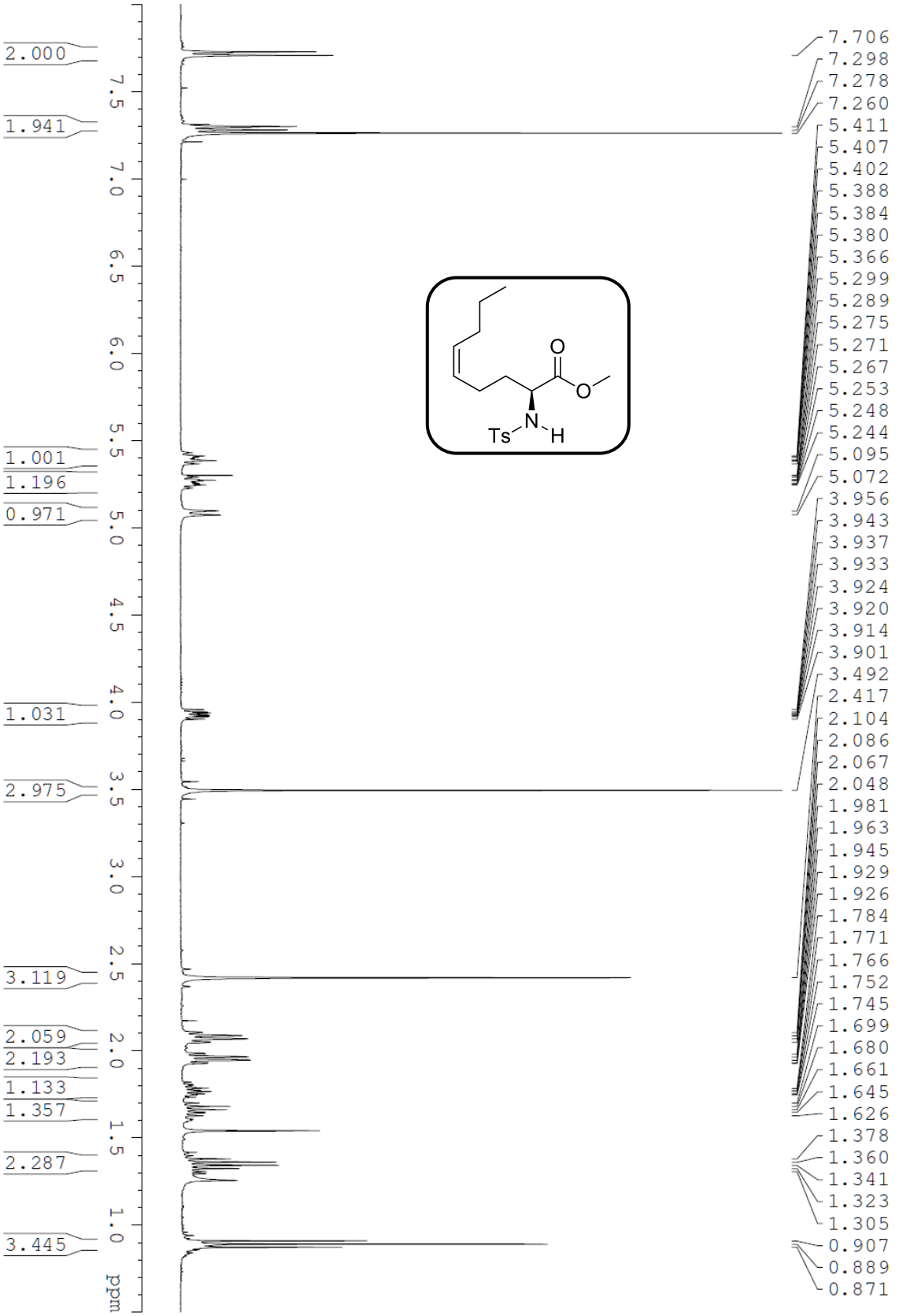

171.615
170.553
150.978
145.487
137.629
130.091
129.665
86.398
78.321
78.003
77.685
56.472
53.749
53.082
37.489
28.788
22.637
O
O
O
O
Ts
N
Boc
1a

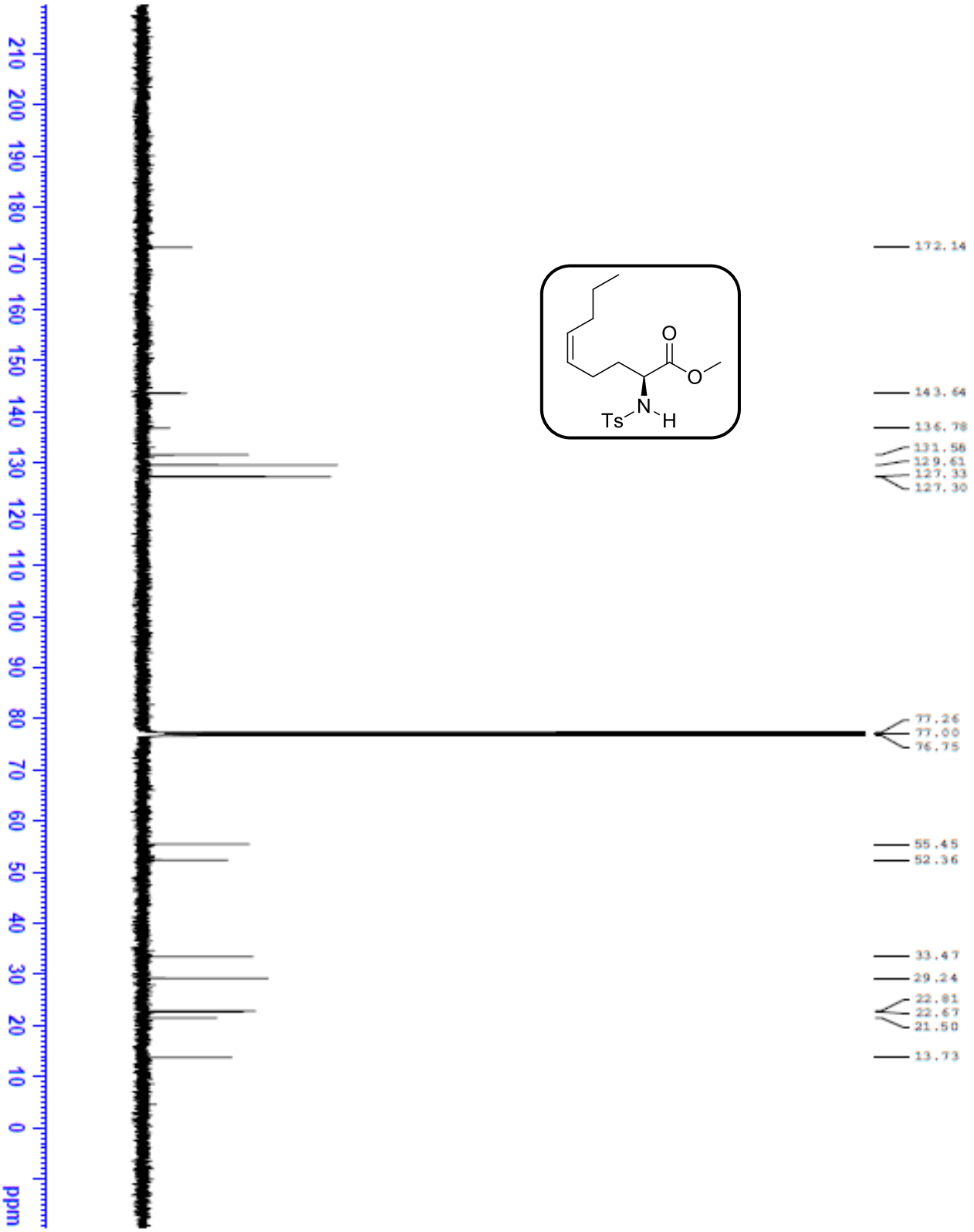

2.000
2.099
0.973
1.029
3.110
3.110
1.016
1.005
3.064
7.755
7.735
7.313
7.293
7.260
5.596
5.578
4.170
4.159
4.149
4.140
4.129
3.666
3.598
2.994
2.983
2.951
2.941
2.877
2.865
2.834
2.822
2.424
O
O
O
O
Ts
N
H
2a
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm

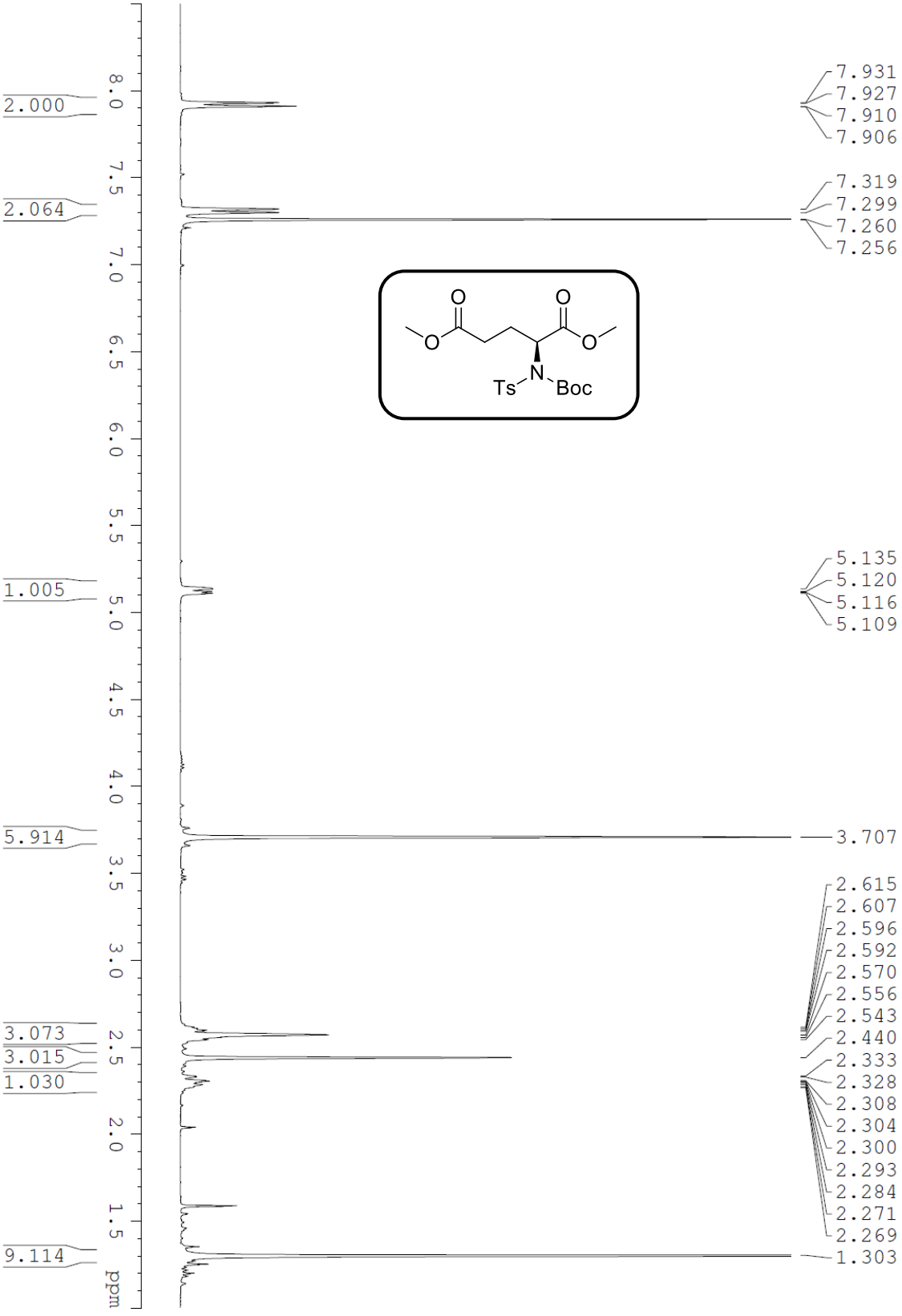

171.662
171.075
148.588
135.432
134.561
133.873
131.407
126.502
78.316
77.998
77.681
54.032
53.836
53.196
38.526
2a
Ts
N
H
O
ppm

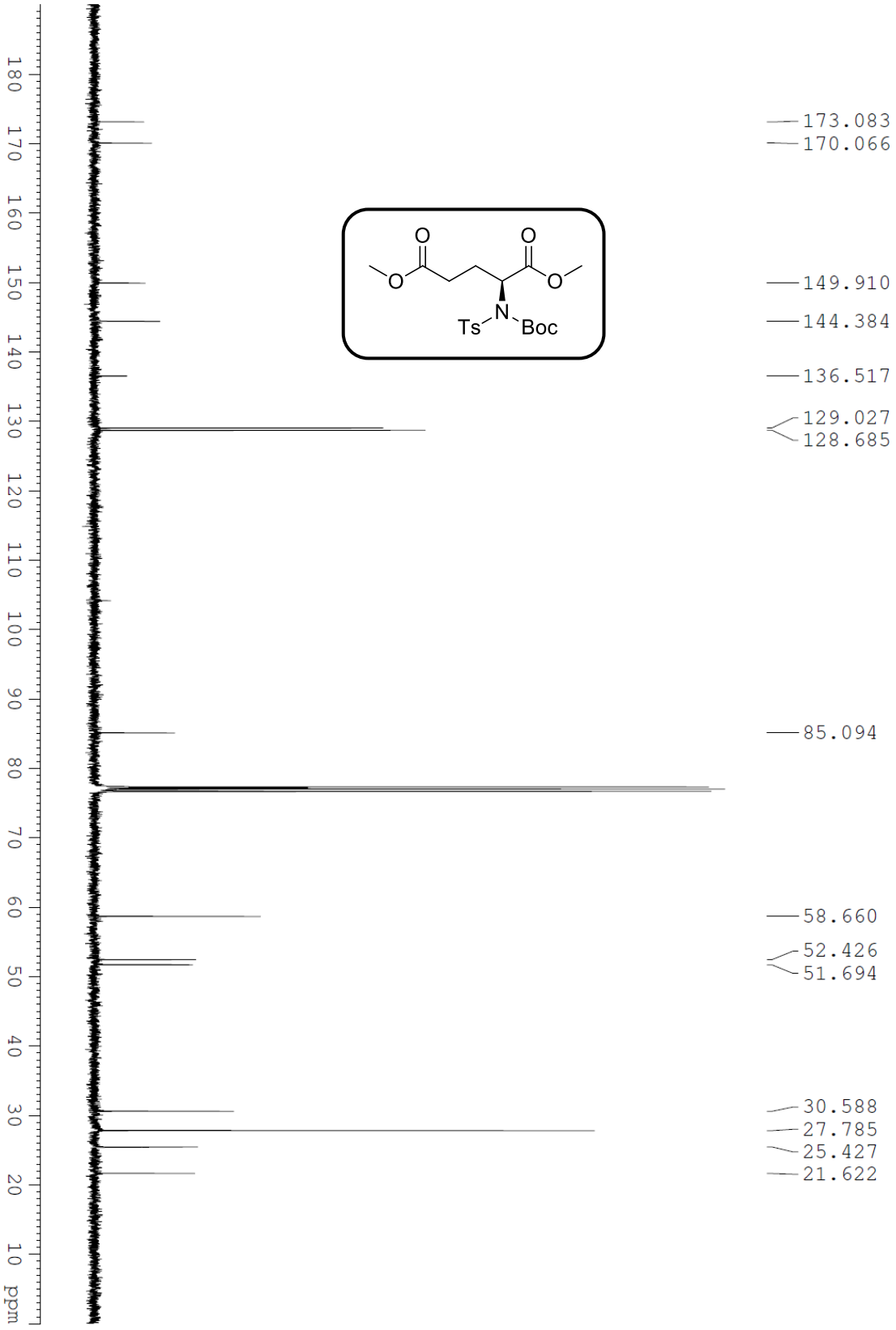

7.931
7.324
7.303
7.260
5.454
5.442
5.430
5.096
5.089
5.084
5.073
5.067
5.061
3.721
2.446
2.288
2.277
2.262
2.257
2.253
2.244
2.238
2.227
2.062
2.055
2.044
2.037
2.023
2.009
2.006
1.989
1.405
1.386
1.368
1.356
1.349
2.110
1.841
0.961
2.991
3.017
3.030
3.272
2.176
9.235
3.099
O
O
N
Ts
Boc
ppm

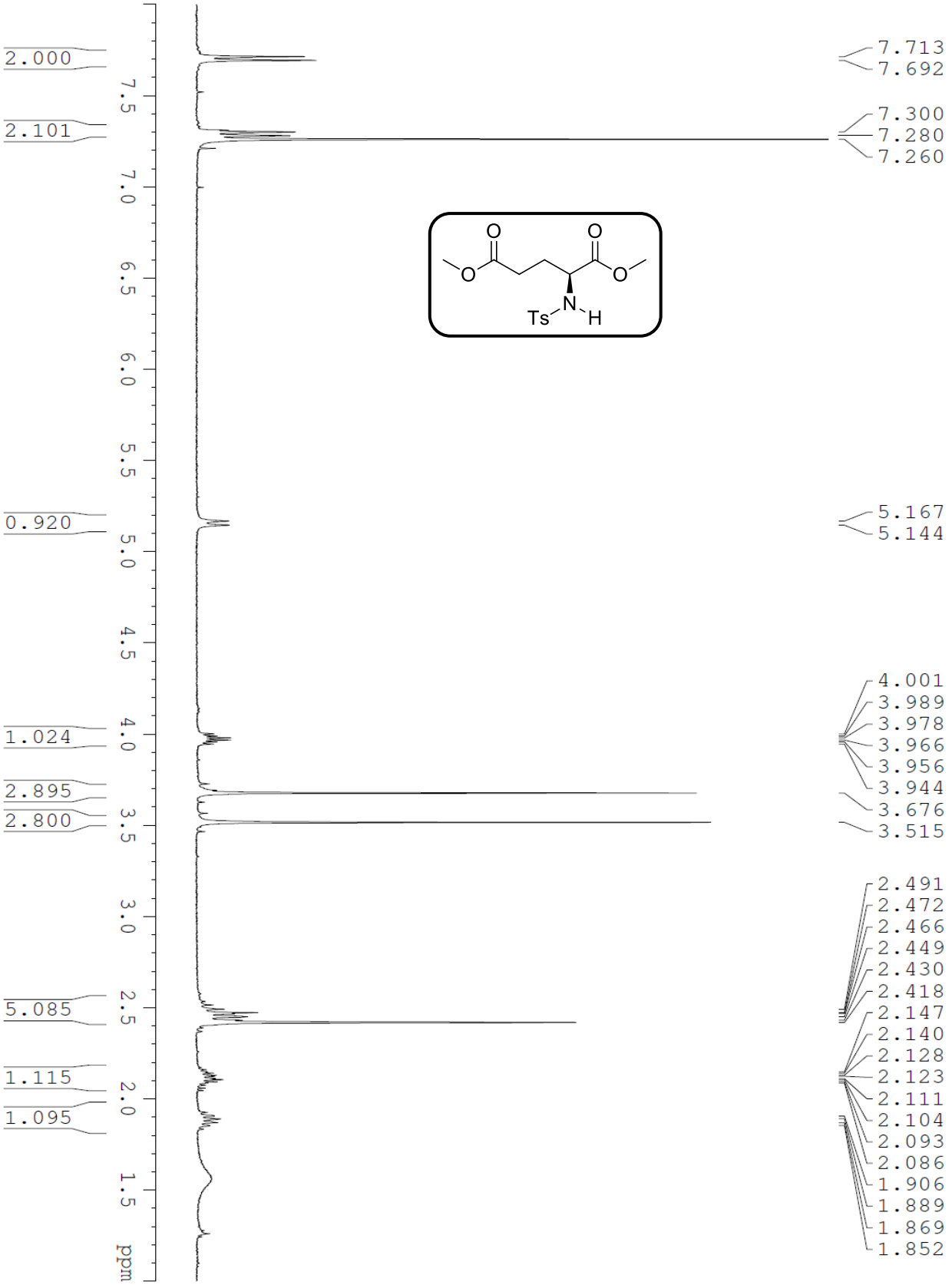

170.60
150.00
144.26
136.78
131.21
129.02
128.69
128.05
84.82
59.05
52.35
30.59
29.28
28.25
27.80
24.39
22.76
21.63
13.75
O
O
N
Ts
Boc
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

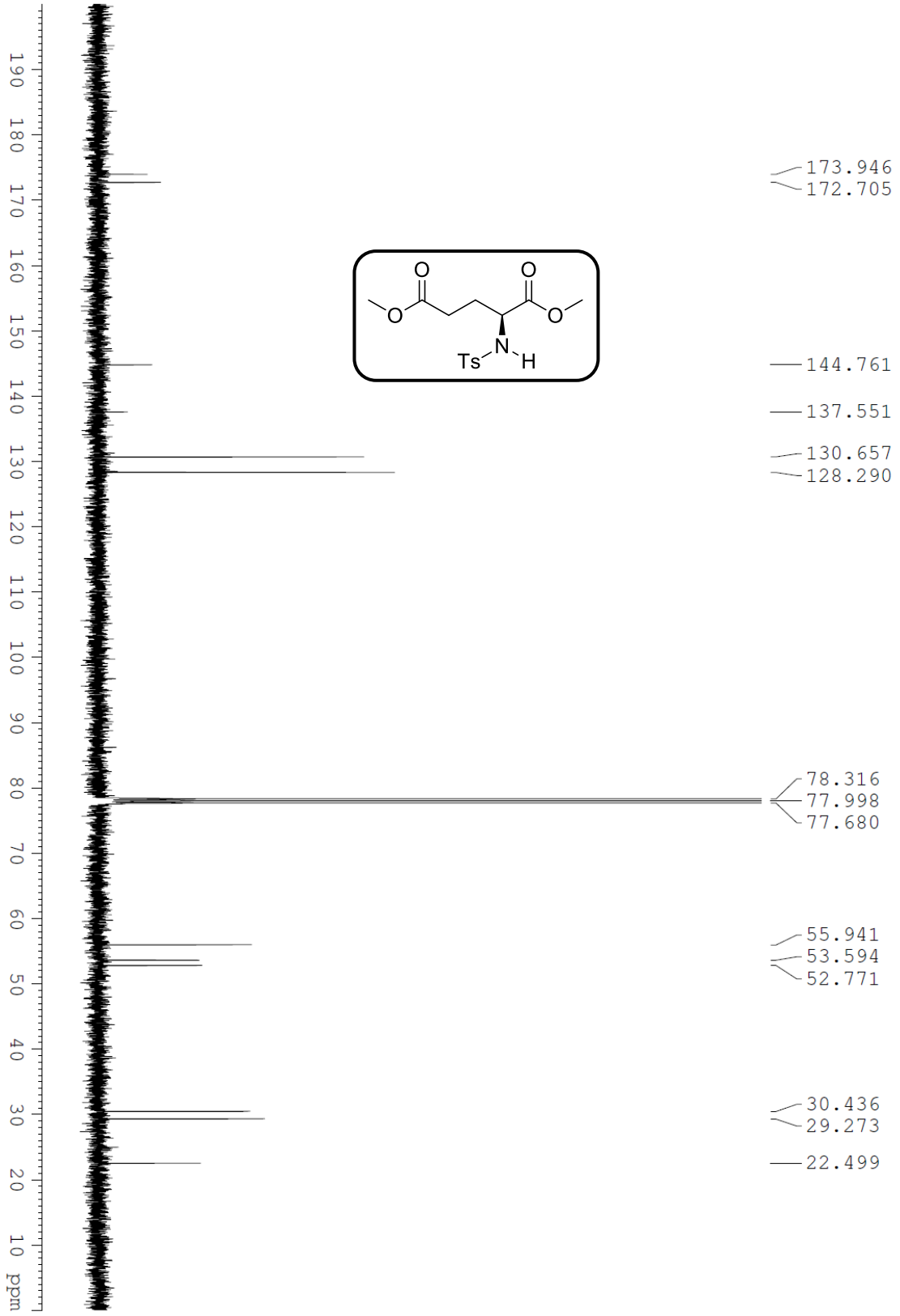

2.000
1.941
1.001
1.196
0.971
1.031
2.975
3.119
2.059
2.193
1.133
1.357
2.287
3.445
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
O
O
Ts
N
H
7.706
7.298
7.278
7.260
5.411
5.407
5.402
5.388
5.384
5.380
5.366
5.299
5.289
5.275
5.271
5.267
5.253
5.248
5.244
5.095
5.072
3.956
3.943
3.937
3.933
3.924
3.920
3.914
3.901
3.492
2.417
2.104
2.086
2.067
2.048
1.981
1.963
1.945
1.929
1.926
1.784
1.771
1.766
1.752
1.745
1.699
1.680
1.661
1.645
1.626
1.378
1.360
1.341
1.323
1.305
0.907
0.889
0.871

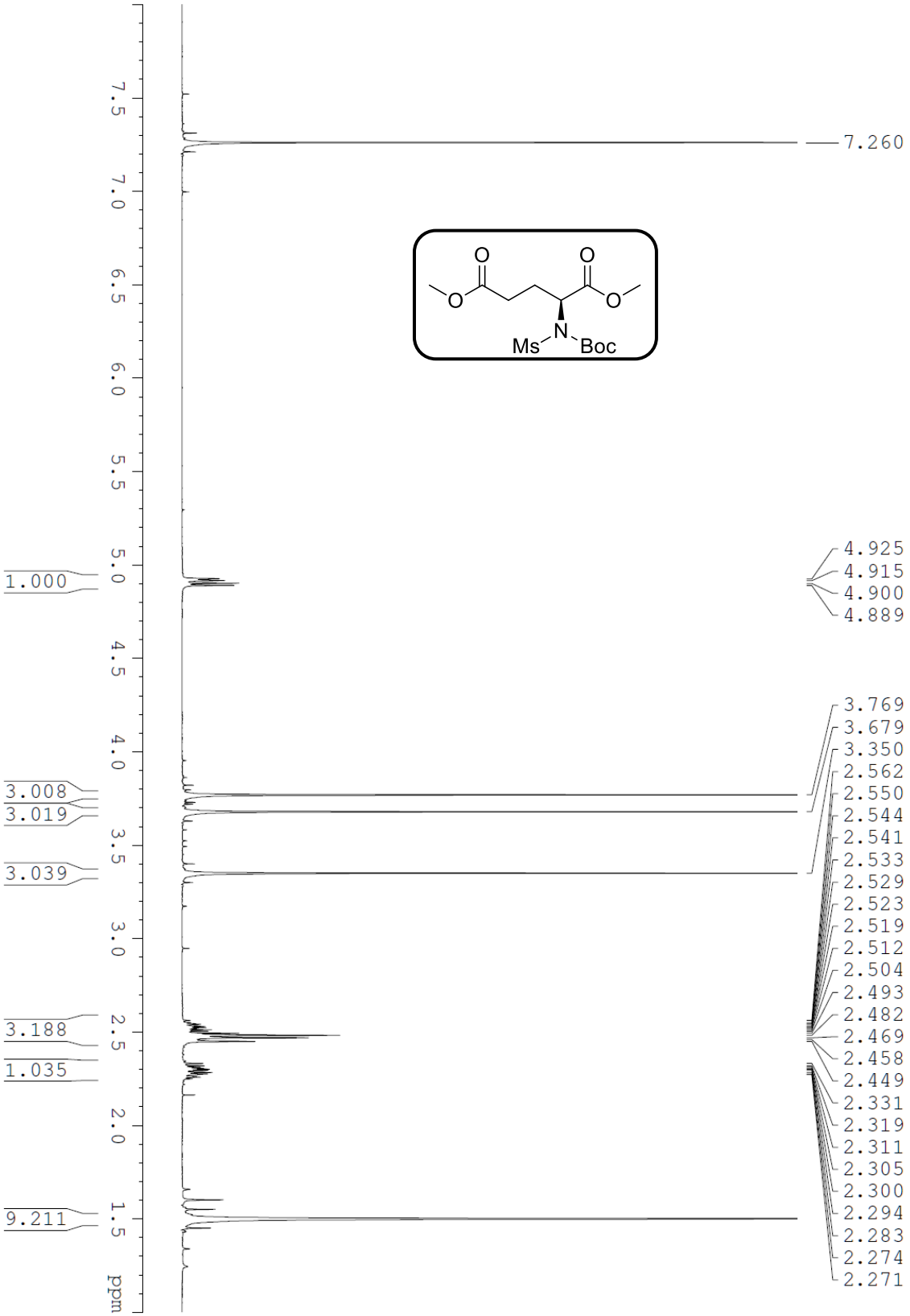

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
O
O
N
H
Ts
172.14
143.64
136.78
131.58
129.61
127.33
127.30
77.26
77.00
76.75
55.45
52.36
33.47
29.24
22.81
22.67
21.50
13.73

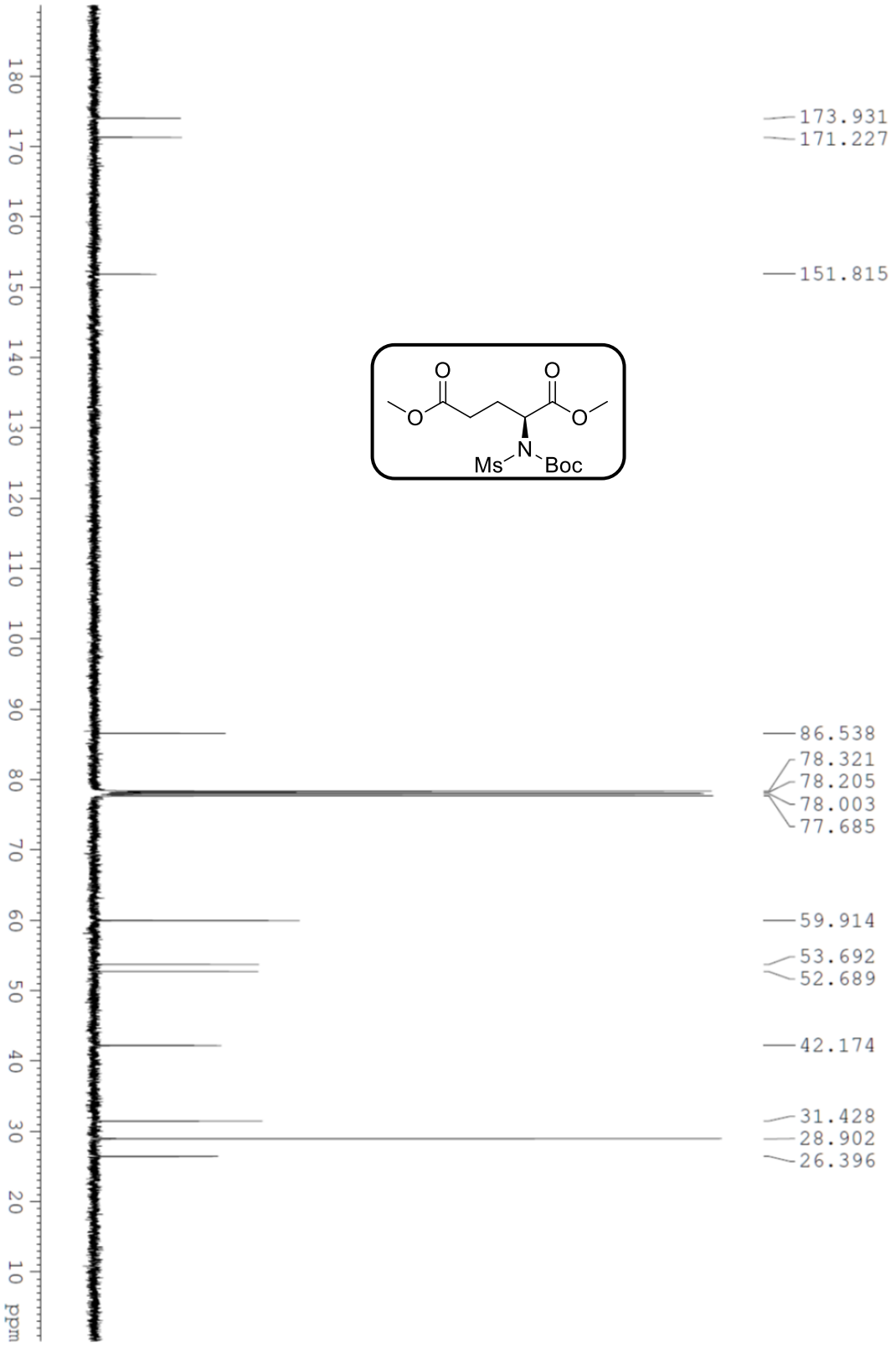

7.931
7.927
7.910
7.906
7.319
7.299
7.260
7.256
5.135
5.120
5.116
5.109
3.707
2.615
2.607
2.596
2.592
2.570
2.556
2.543
2.440
2.333
2.328
2.308
2.304
2.300
2.293
2.284
2.271
2.269
1.303
2.000
2.064
1.005
5.914
3.073
3.015
1.030
9.114
ppm
O
O
O
O
N
Ts
Boc

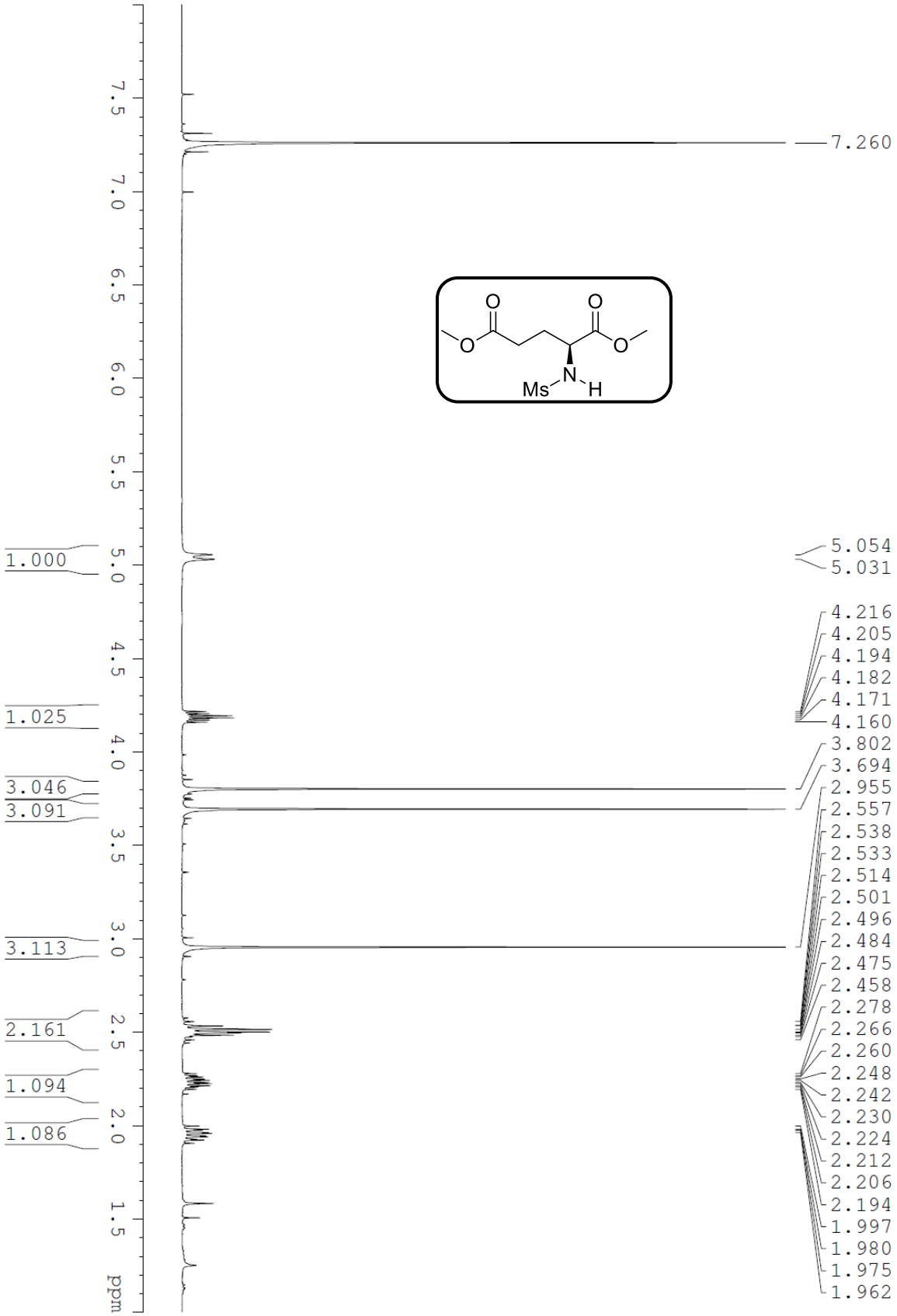

173.083
170.066
149.910
144.384
136.517
129.027
128.685
85.094
58.660
52.426
51.694
30.588
27.785
25.427
21.622
Ts
N
Boc
O
O
O
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

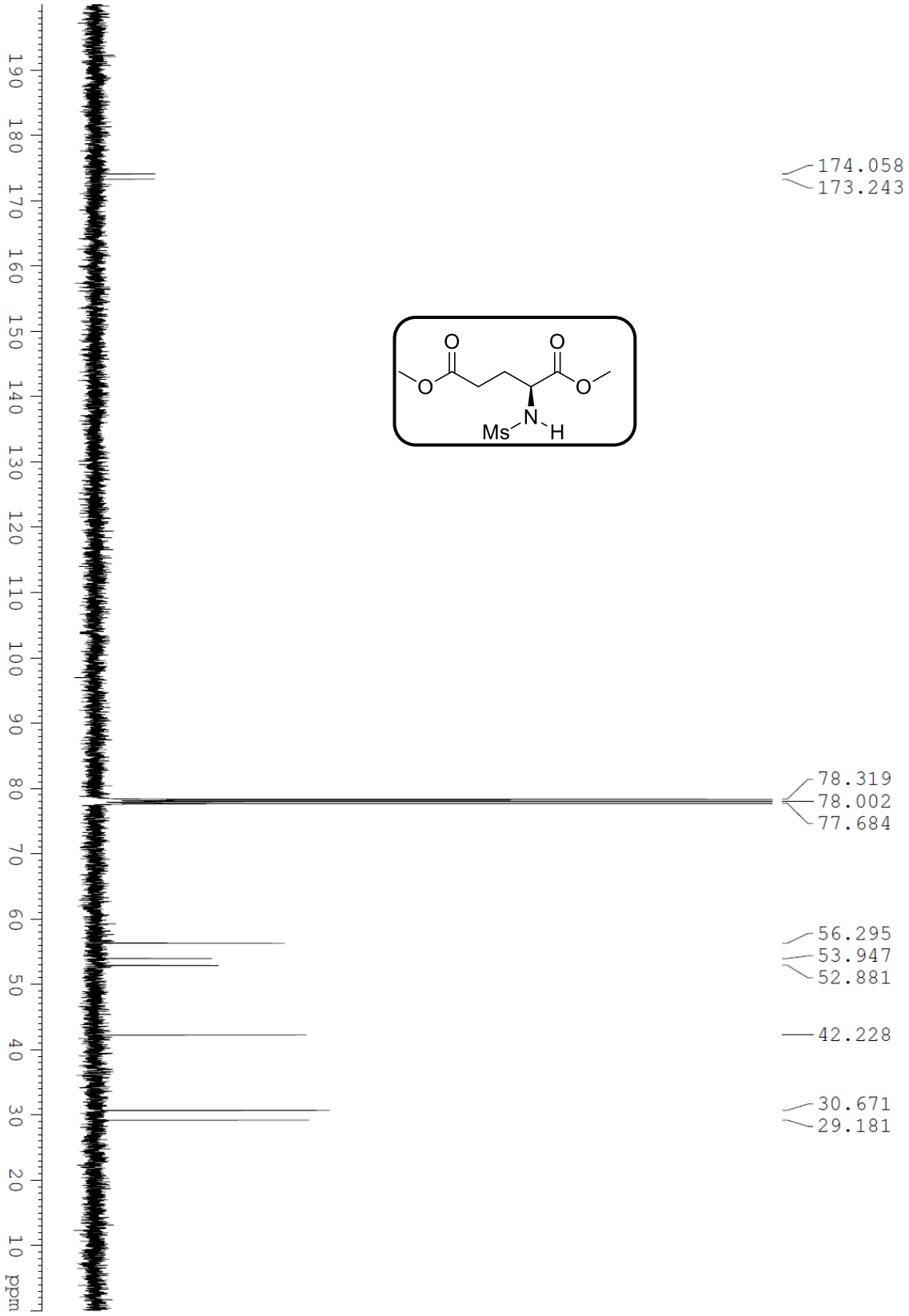

2.000
2.101
0.920
1.024
2.895
2.800
5.085
1.115
1.095
7.713
7.692
7.300
7.280
7.260
5.167
5.144
4.001
3.989
3.978
3.966
3.956
3.944
3.676
3.515
2.491
2.472
2.466
2.449
2.430
2.418
2.147
2.140
2.128
2.123
2.111
2.104
2.093
2.086
1.906
1.889
1.869
1.852
O
O
O
O
N
H
Ts
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm

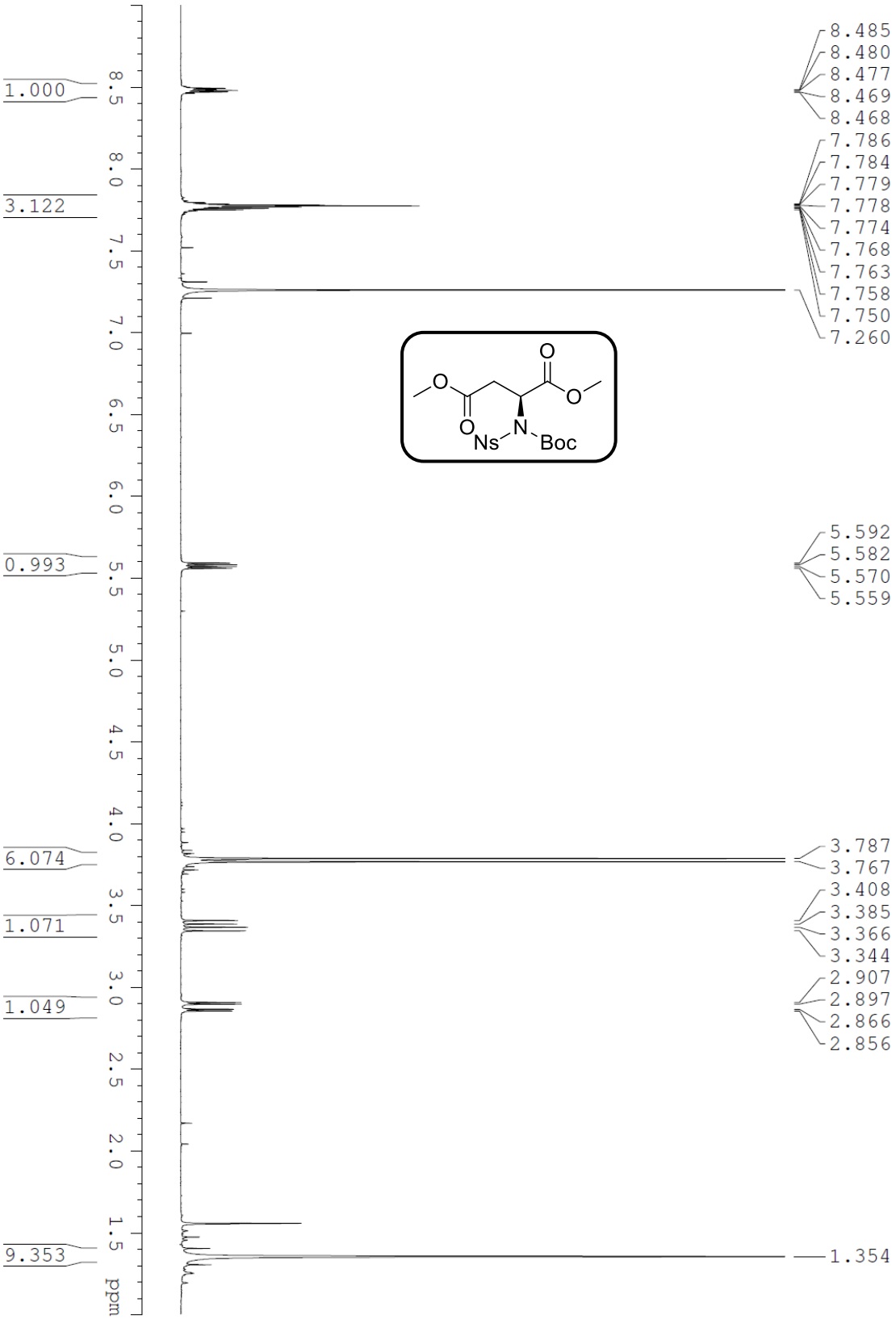

173.946
172.705
144.761
137.551
130.657
128.290
78.316
77.998
77.680
55.941
53.594
52.771
30.436
29.273
22.499
O
O
O
O
N
H
Ts
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

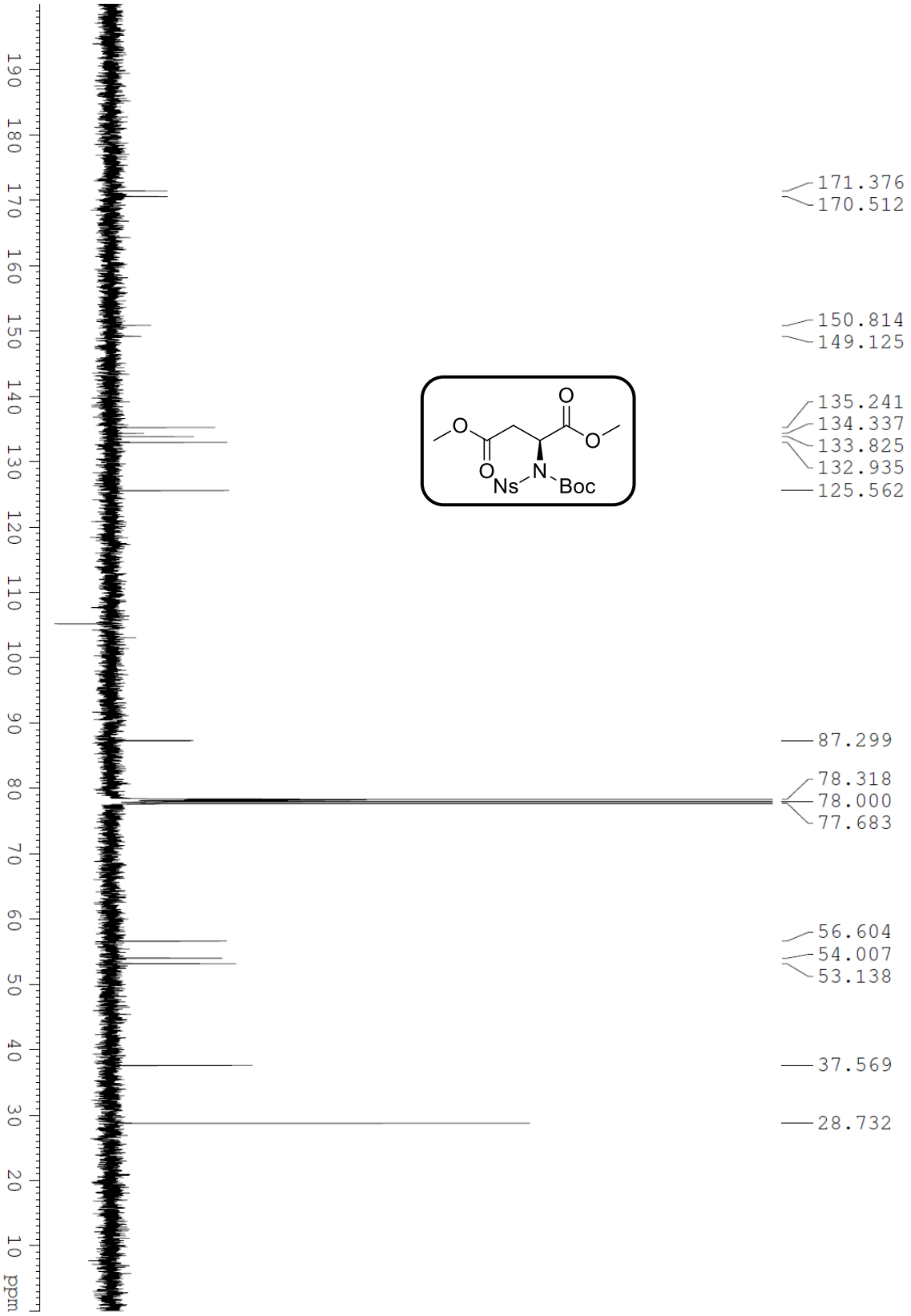

7.260
4.925
4.915
4.900
4.889
3.769
3.679
3.350
2.562
2.550
2.544
2.541
2.533
2.529
2.523
2.519
2.512
2.504
2.493
2.482
2.469
2.458
2.449
2.331
2.319
2.311
2.305
2.300
2.294
2.283
2.274
2.271
1.000
3.008
3.019
3.039
3.188
1.035
9.211
O
O
O
O
N
Ms
Boc
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm

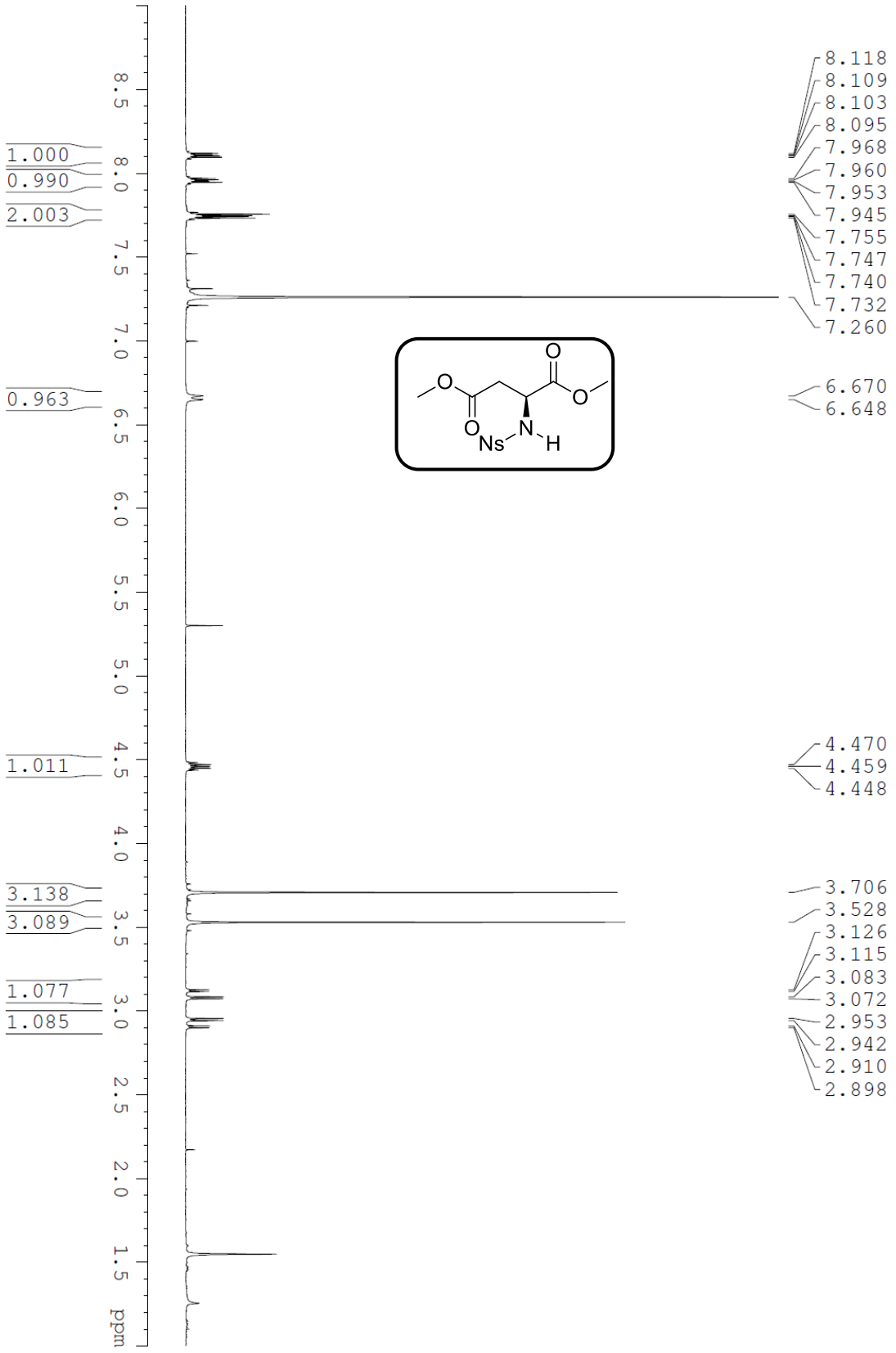

173.931
171.227
151.815
86.538
78.321
78.205
78.003
77.685
59.914
53.692
52.689
42.174
31.428
28.902
26.396
O
O
O
O
N
Ms
Boc
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

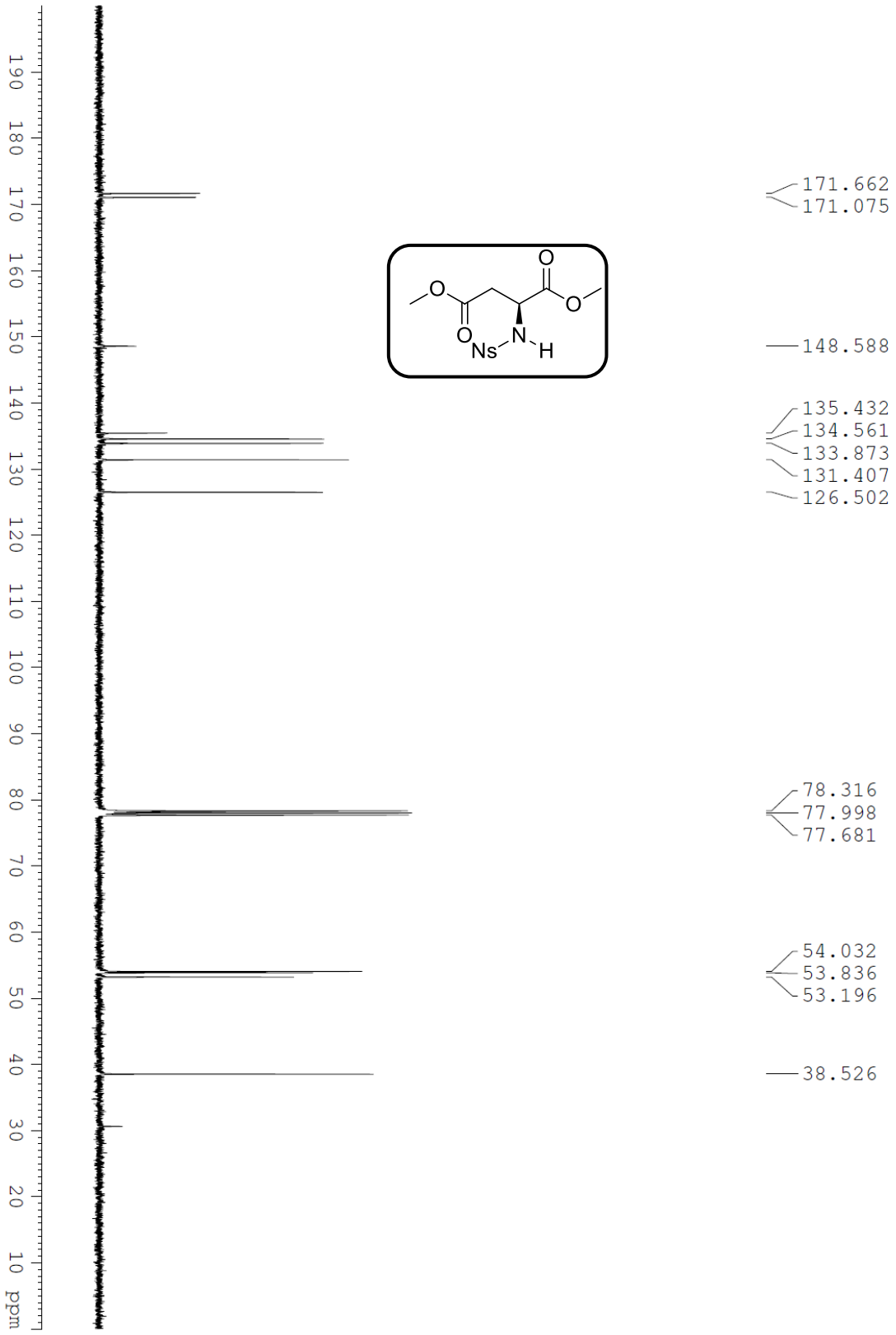

7.260
5.054
5.031
4.216
4.205
4.194
4.182
4.171
4.160
3.802
3.694
2.955
2.557
2.538
2.533
2.514
2.501
2.496
2.484
2.475
2.458
2.278
2.266
2.260
2.248
2.242
2.230
2.224
2.212
2.206
2.194
1.997
1.980
1.975
1.962
1.000
1.025
3.046
3.091
3.113
2.161
1.094
1.086
O
O
O
O
N
H
Ms
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm

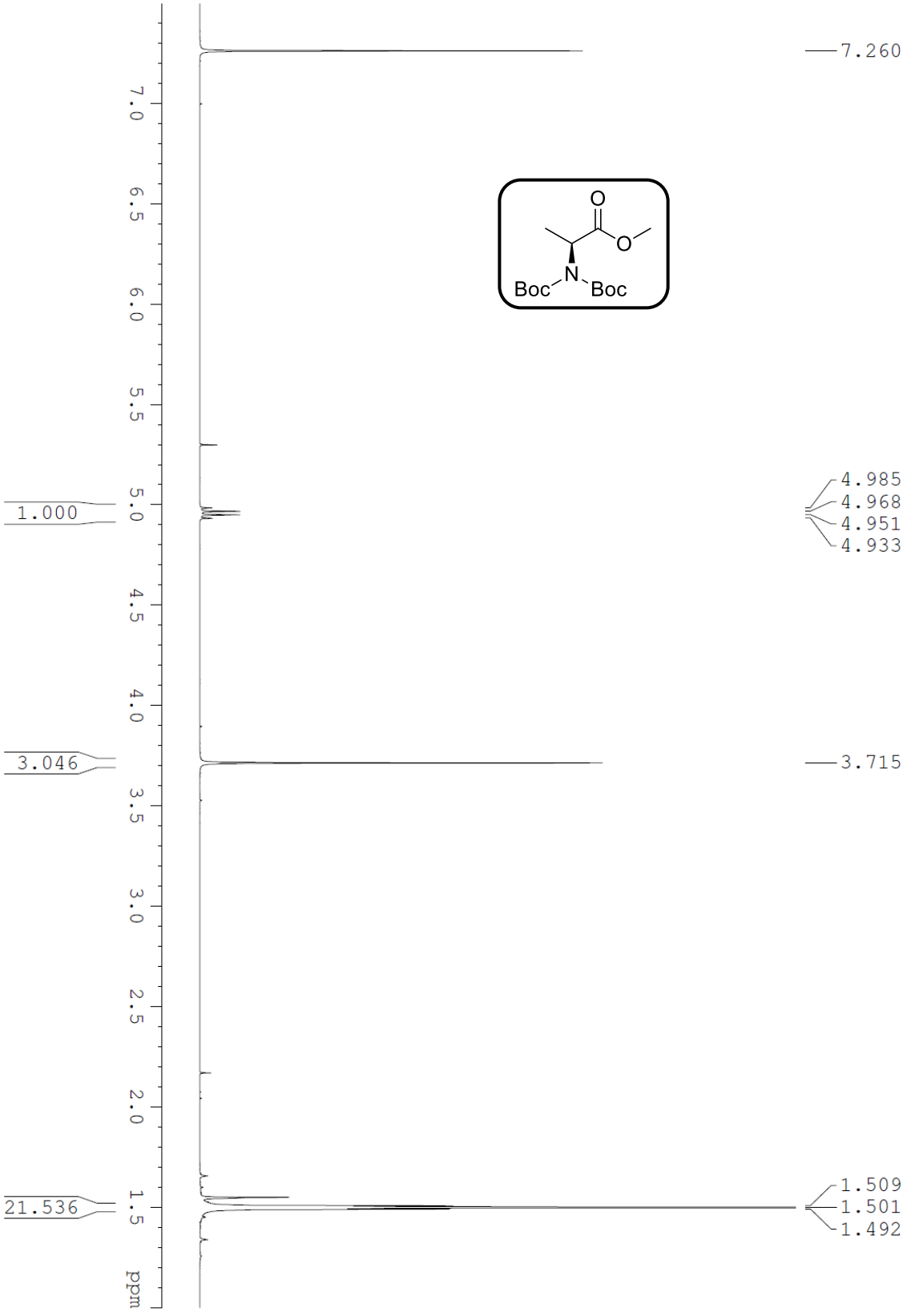

174.058
173.243
78.319
78.002
77.684
56.295
53.947
52.881
42.228
30.671
29.181
O
O
O
O
N
H
Ms
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

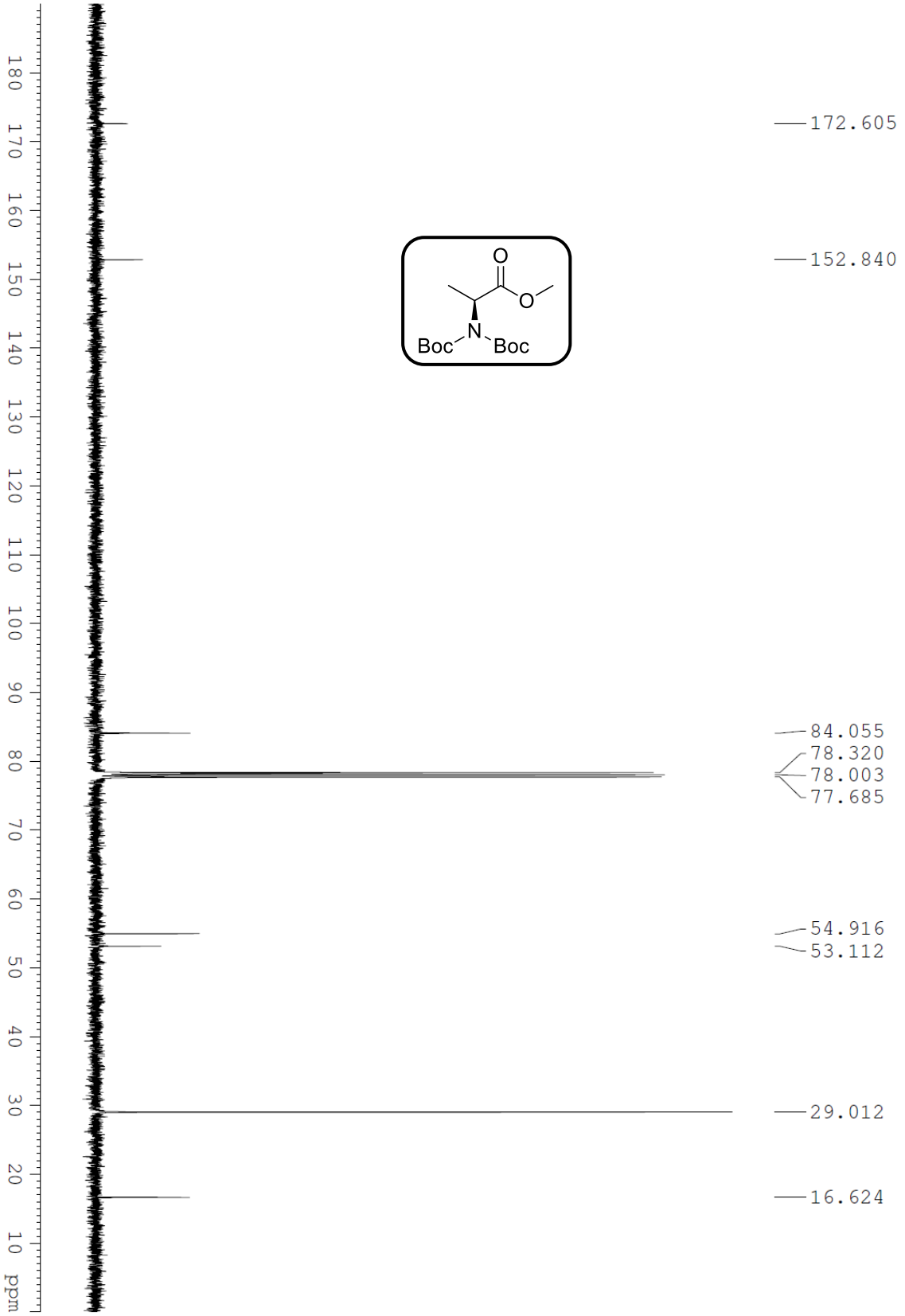

8.485
8.480
8.477
8.469
8.468
7.786
7.784
7.779
7.778
7.774
7.768
7.763
7.758
7.750
7.260
5.592
5.582
5.570
5.559
3.787
3.767
3.408
3.385
3.366
3.344
2.907
2.897
2.866
2.856
1.354
1.000
3.122
0.993
6.074
1.071
1.049
9.353
ppm
O
O
O
O
N
Ns
Boc

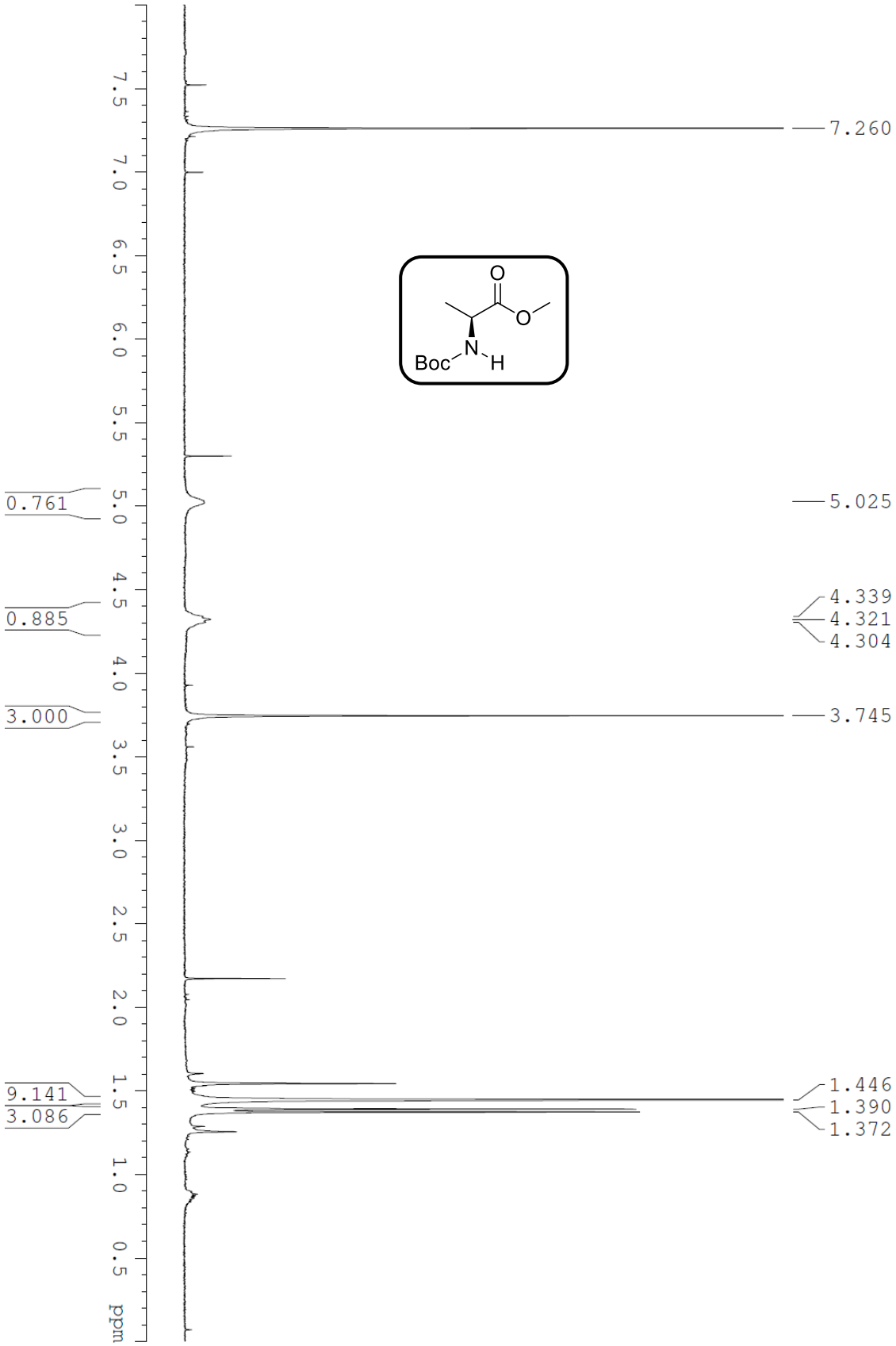

171.376
170.512
150.814
149.125
135.241
134.337
133.825
132.935
125.562
87.299
78.318
78.000
77.683
56.604
54.007
53.138
37.569
28.732
O
O
O
O
N
Ns
Boc
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

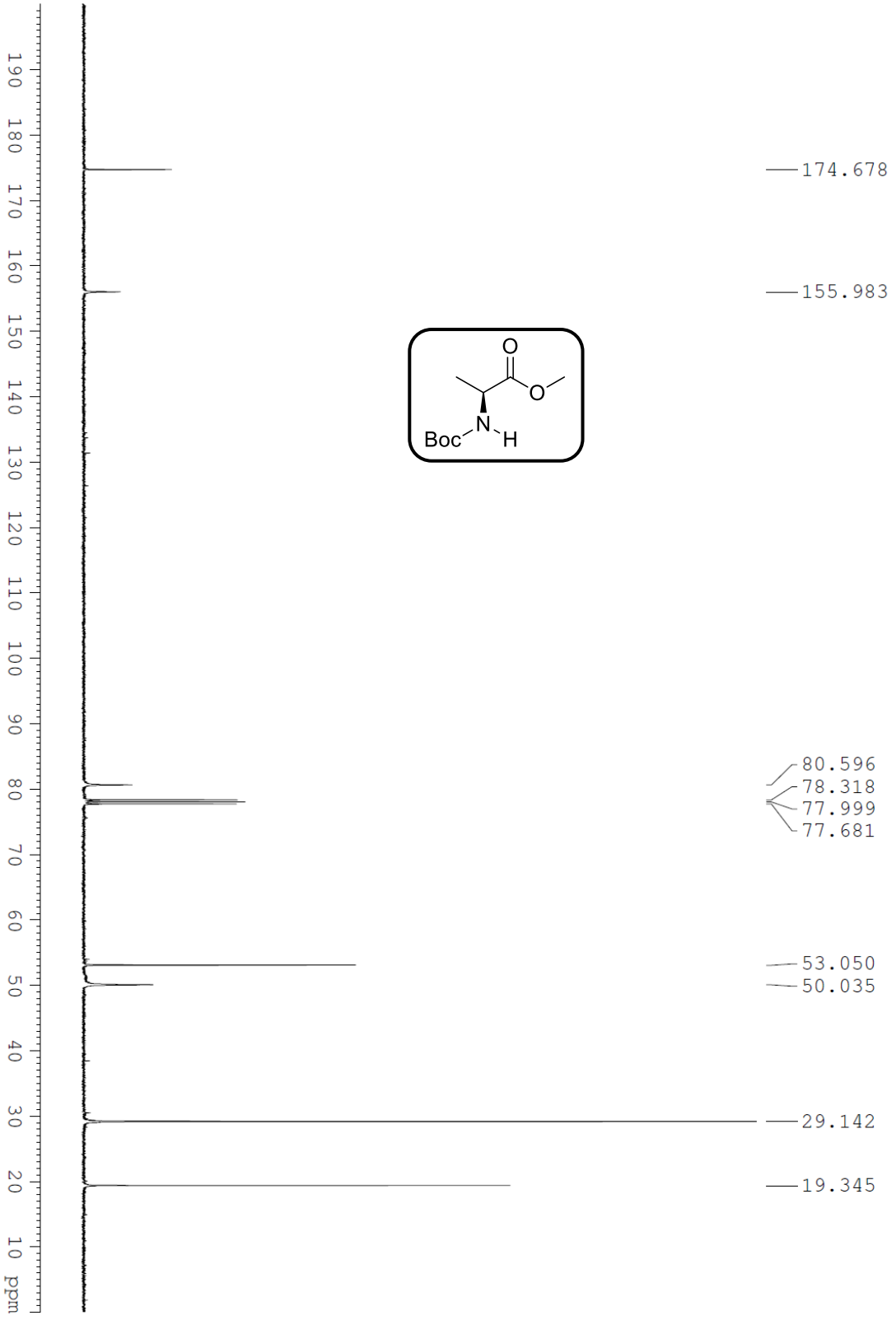

8.118
8.109
8.103
8.095
7.968
7.960
7.953
7.945
7.755
7.747
7.740
7.732
7.260
6.670
6.648
4.470
4.459
4.448
3.706
3.528
3.126
3.115
3.083
3.072
2.953
2.942
2.910
2.898
1.000
0.990
2.003
0.963
1.011
3.138
3.089
1.077
1.085
O
O
O
O
Ns
N
H
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm

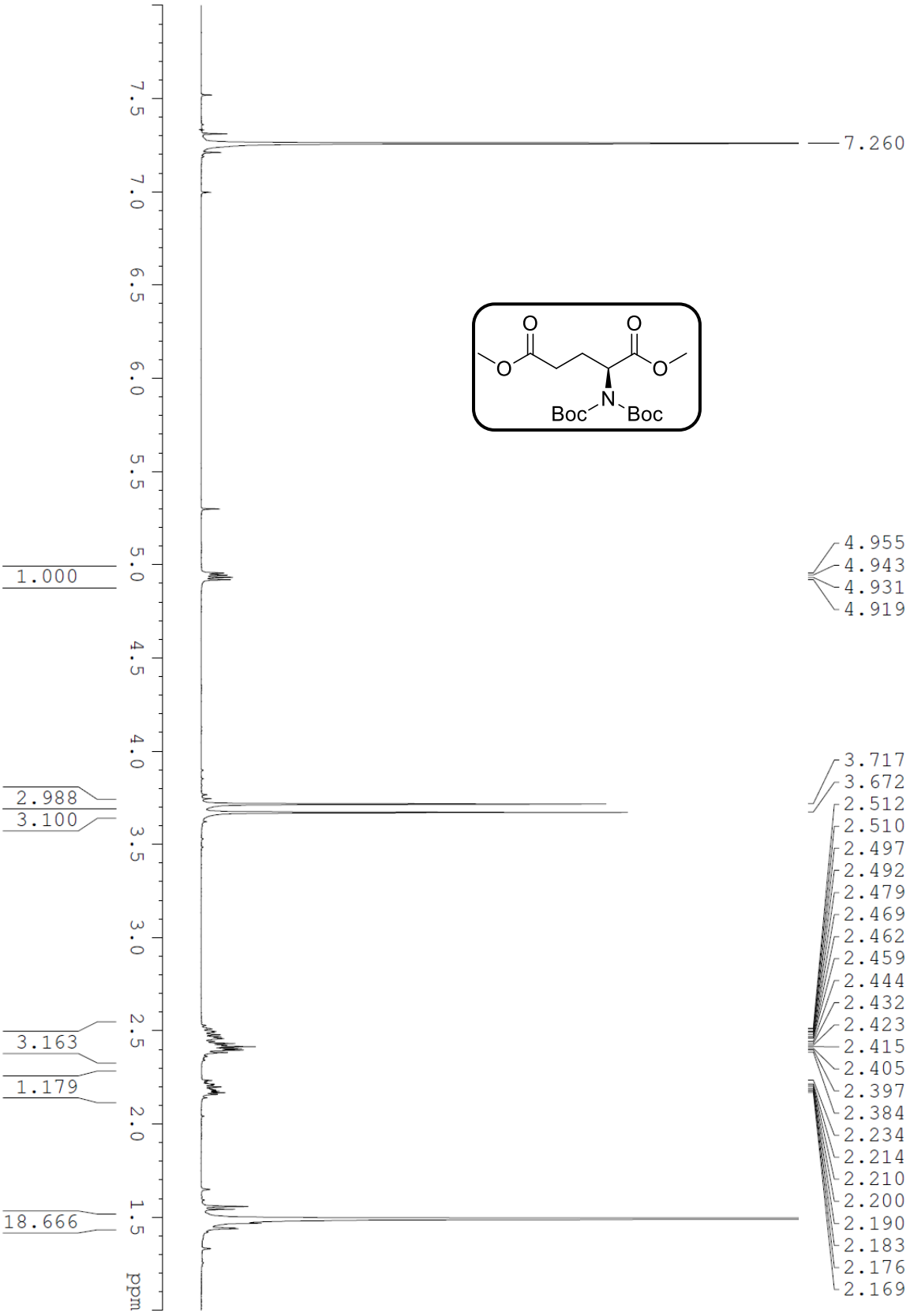

171.662
171.075
148.588
135.432
134.561
133.873
131.407
126.502
78.316
77.998
77.681
54.032
53.836
53.196
38.526
O
O
O
O
Ns
N
H
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

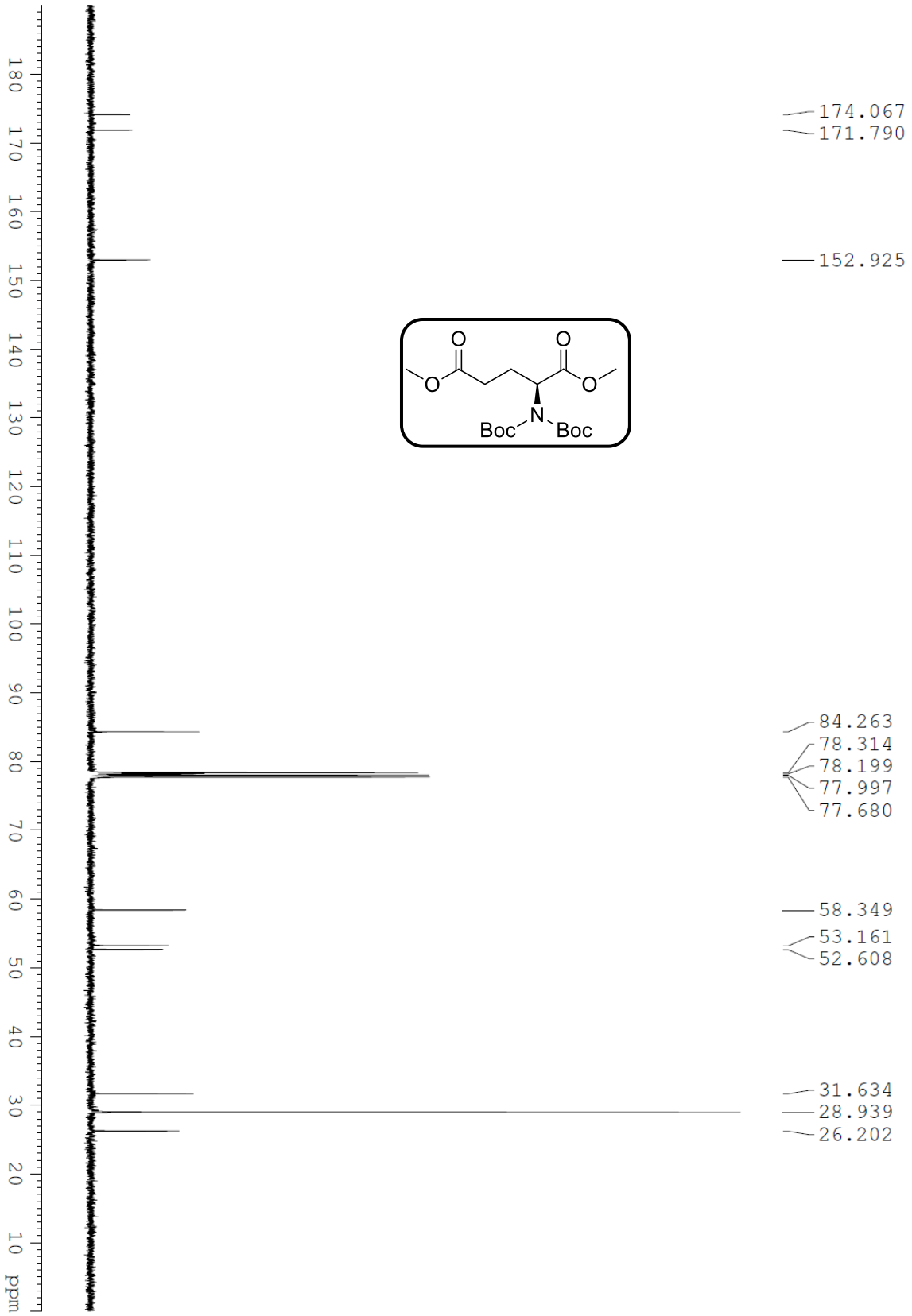

7.260
4.985
4.968
4.951
4.933
3.715
1.509
1.501
1.492
1.000
3.046
21.536
Boc
Boc
N
O
O
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm


172.605
152.840
84.055
78.320
78.003
77.685
54.916
53.112
29.012
16.624
O
O
N
Boc
Boc
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

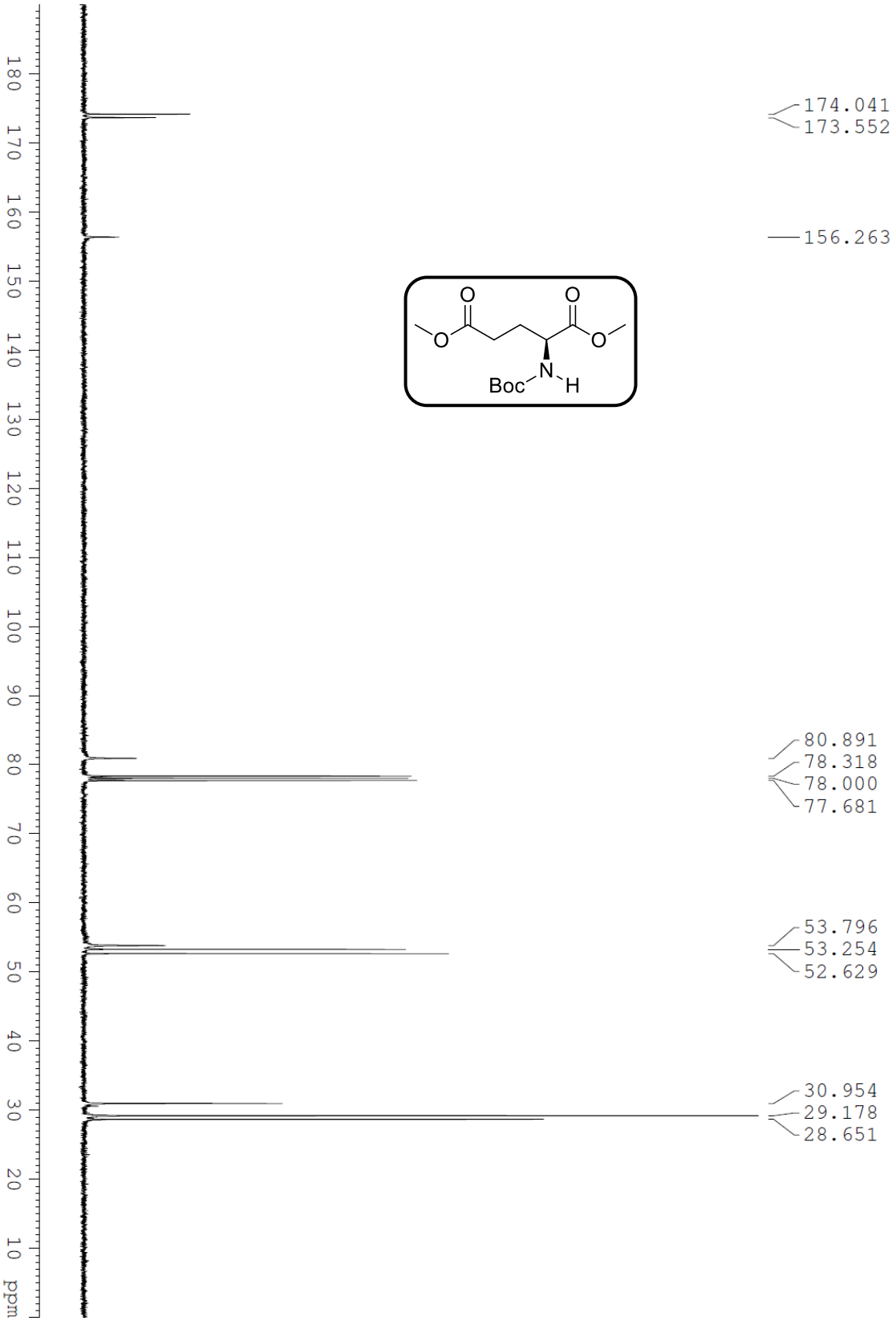

7.260
5.025
4.339
4.321
4.304
3.745
1.446
1.390
1.372
0.761
0.885
3.000
9.141
3.086
Boc
N
H
O
O
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

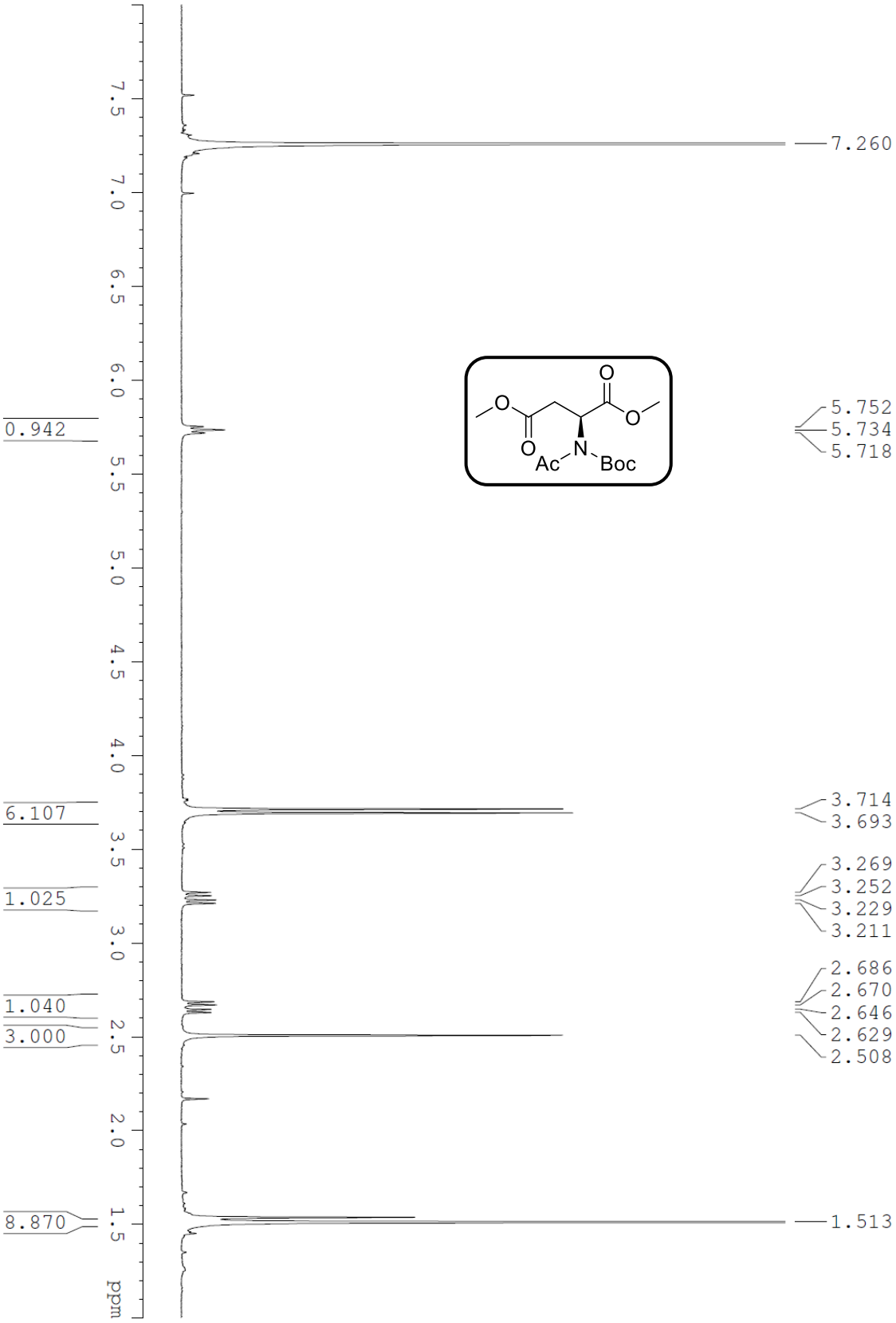

174.678
155.983
80.596
78.318
77.999
77.681
53.050
50.035
29.142
19.345
O
O
N
H
Boc
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

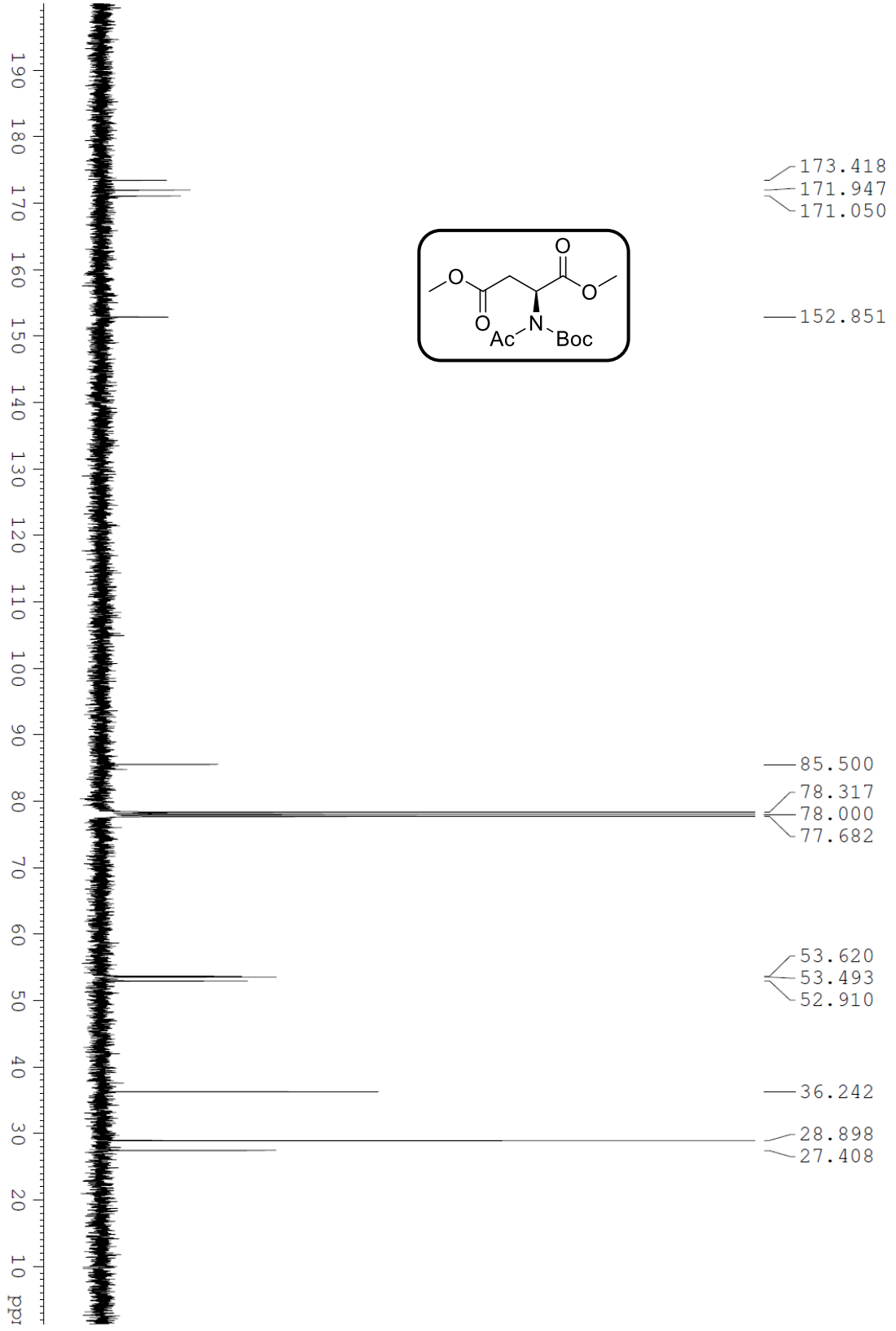

7.260
4.955
4.943
4.931
4.919
3.717
3.672
2.512
2.510
2.497
2.492
2.479
2.469
2.462
2.459
2.444
2.432
2.423
2.415
2.405
2.397
2.384
2.234
2.214
2.210
2.200
2.190
2.183
2.176
2.169
1.000
2.988
3.100
3.163
1.179
18.666
ppm
O
O
O
O
N
Boc
Boc

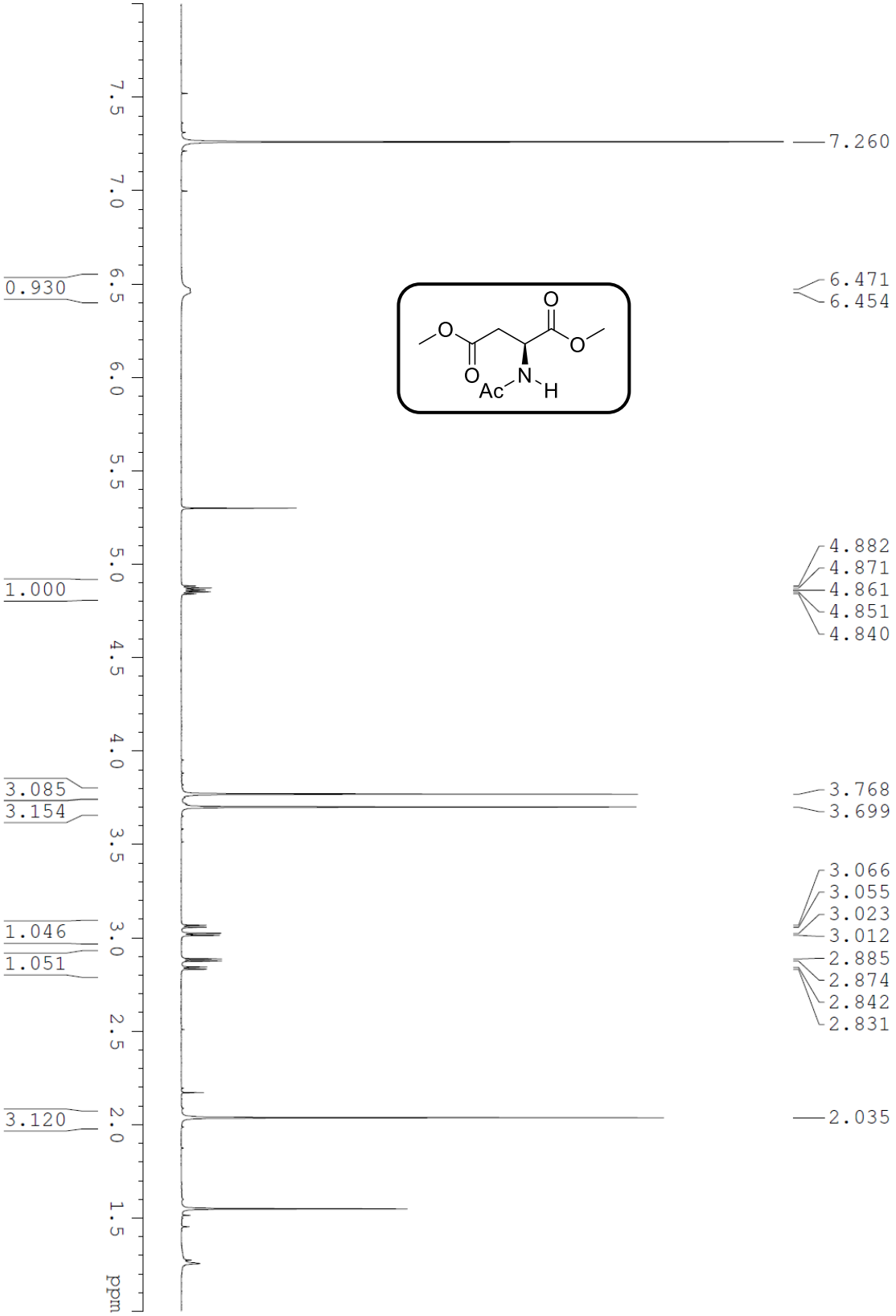

174.067
171.790
152.925
84.263
78.314
78.199
77.997
77.680
58.349
53.161
52.608
31.634
28.939
26.202
O
O
O
O
N
Boc
Boc
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

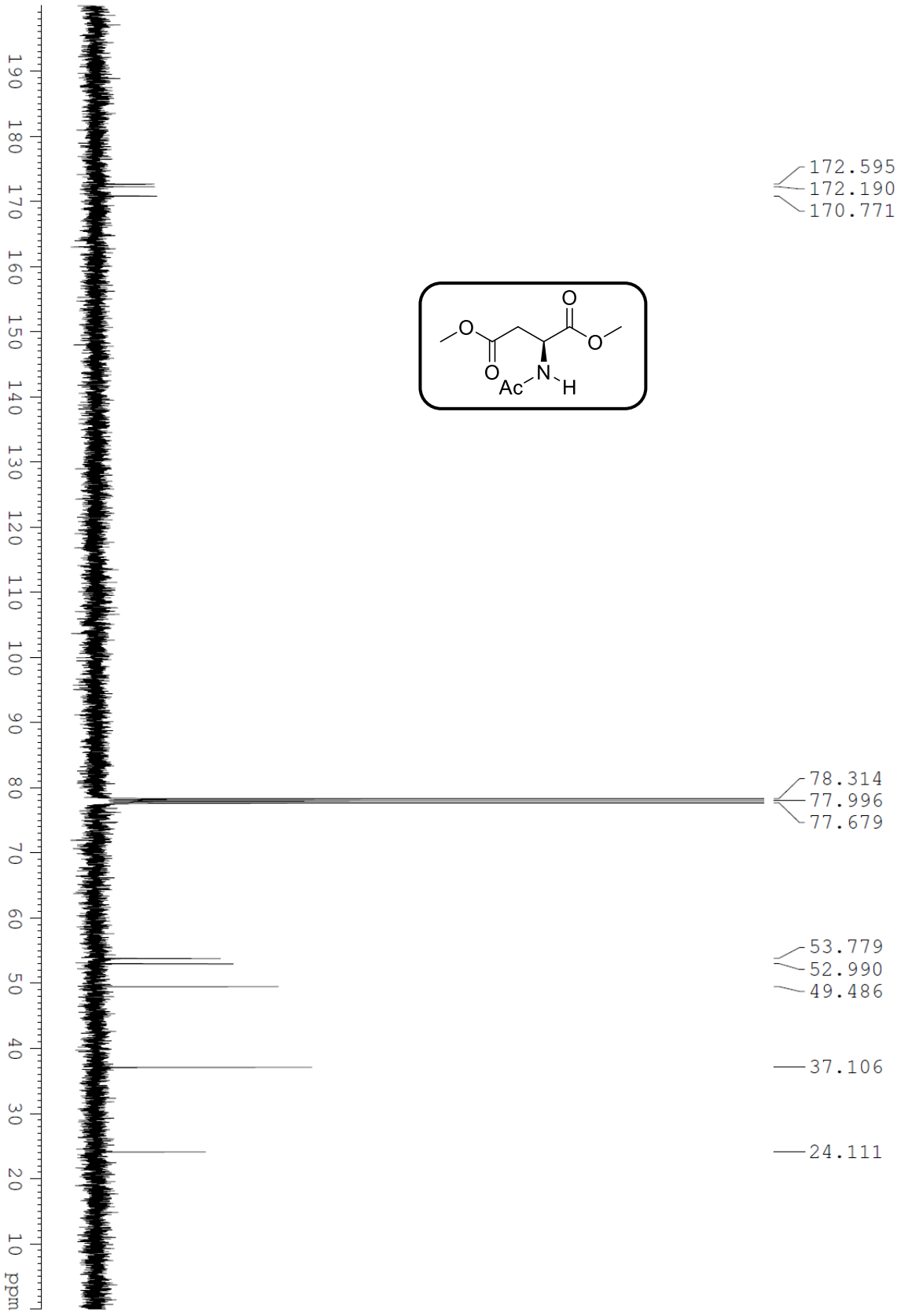

7.260
5.099
5.083
4.349
4.335
3.748
3.681
2.462
2.439
2.420
2.400
2.381
2.358
2.339
2.230
2.212
2.196
2.173
2.171
2.170
2.163
2.145
2.033
1.998
1.978
1.962
1.942
1.926
0.817
0.883
3.000
3.009
2.124
1.151
1.102
9.106
Boc
N
H
O
O
O
O
ppm


174.041
173.552
156.263
80.891
78.318
78.000
77.681
53.796
53.254
52.629
30.954
29.178
28.651
O
O
O
O
N
H
Boc
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

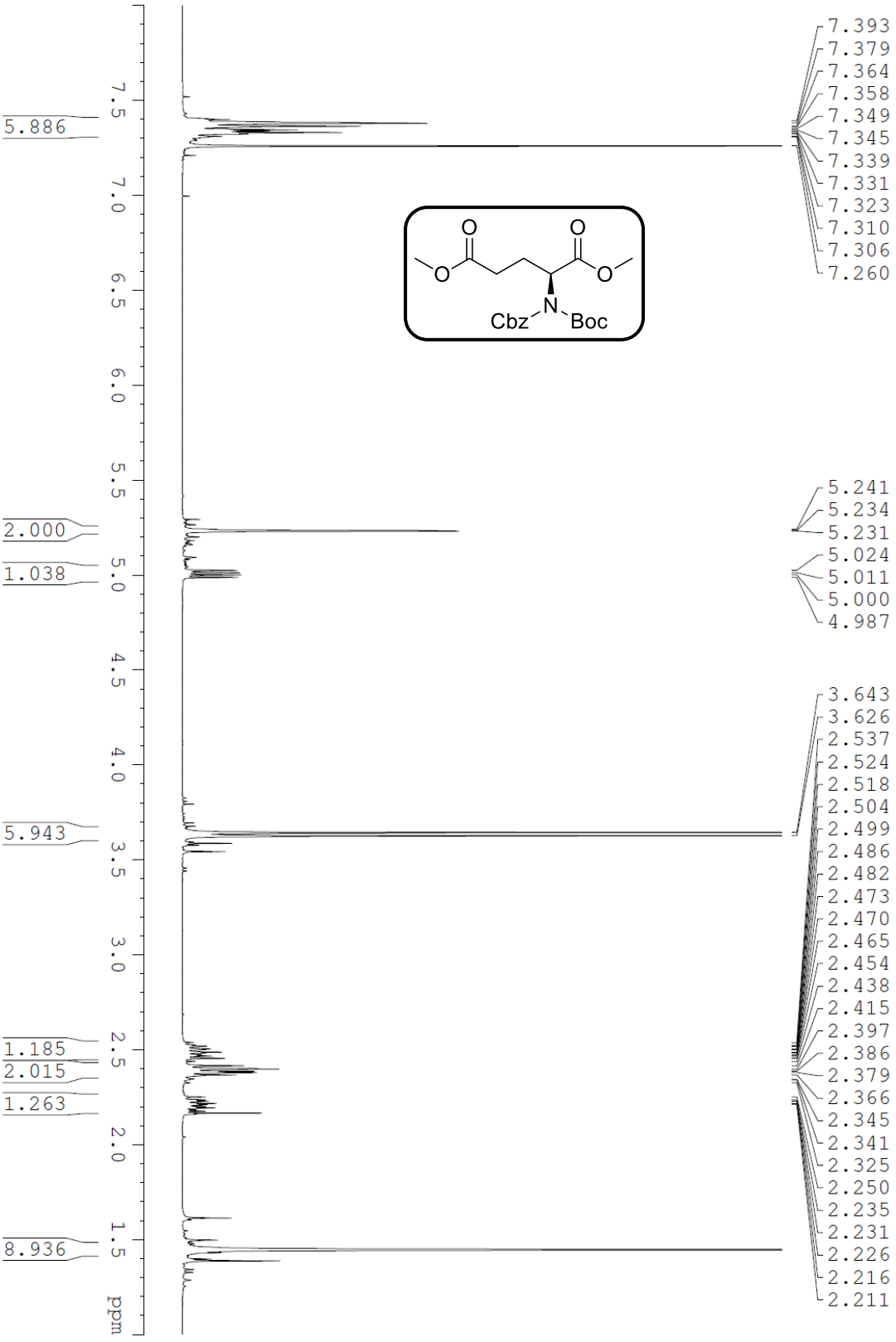

7.260
5.752
5.734
5.718
3.714
3.693
3.269
3.252
3.229
3.211
2.686
2.670
2.646
2.629
2.508
1.513
0.942
6.107
1.025
1.040
3.000
8.870
Ac
N
Boc
ppm

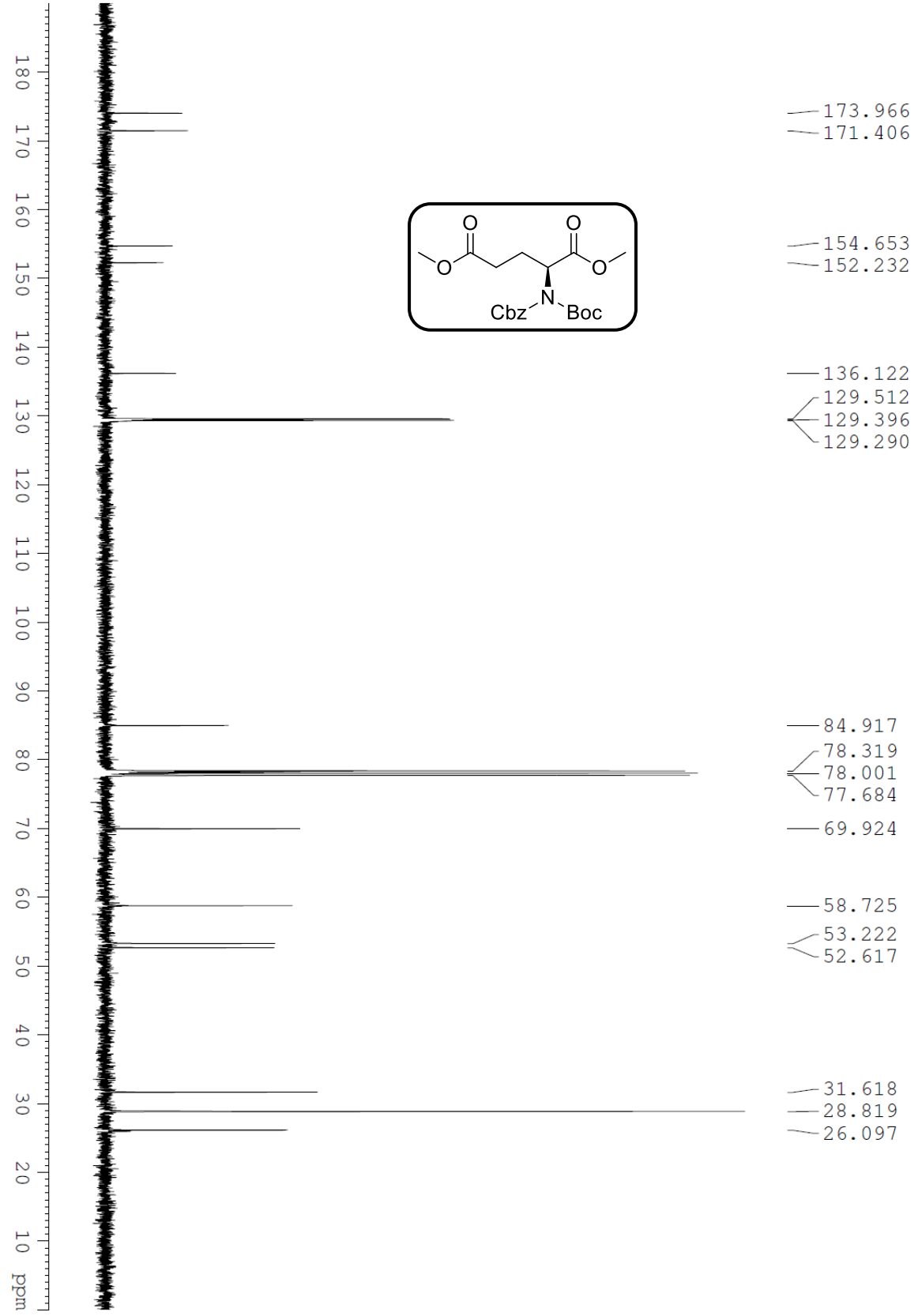

173.418
171.947
171.050
152.851
85.500
78.317
78.000
77.682
53.620
53.493
52.910
36.242
28.898
27.408
O
O
O
O
N
Ac
Boc
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.260
6.471
6.454
4.882
4.871
4.861
4.851
4.840
3.768
3.699
3.066
3.055
3.023
3.012
2.885
2.874
2.842
2.831
2.035
0.930
1.000
3.085
3.154
1.046
1.051
3.120
O
O
O
O
Ac
N
H
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm

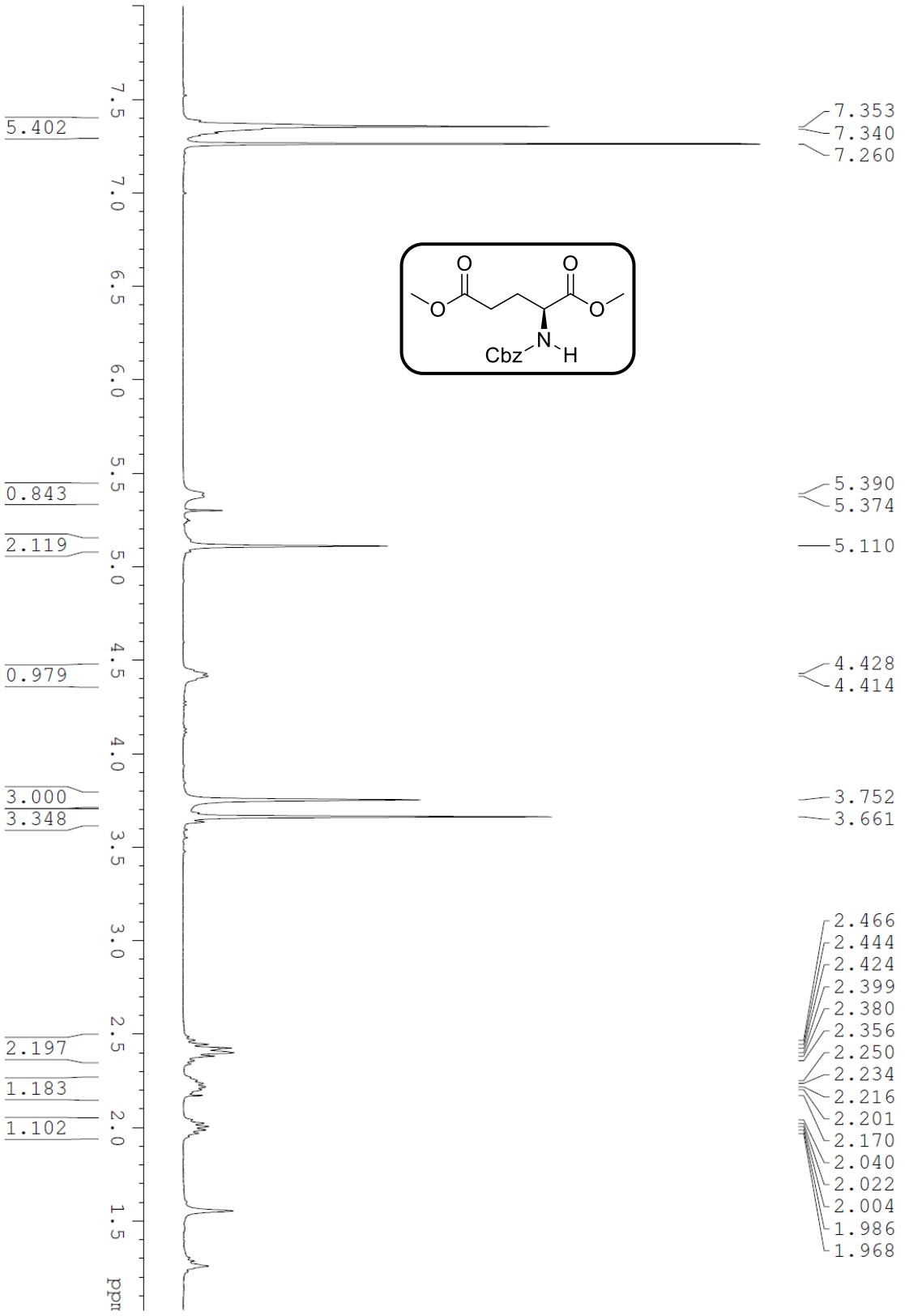


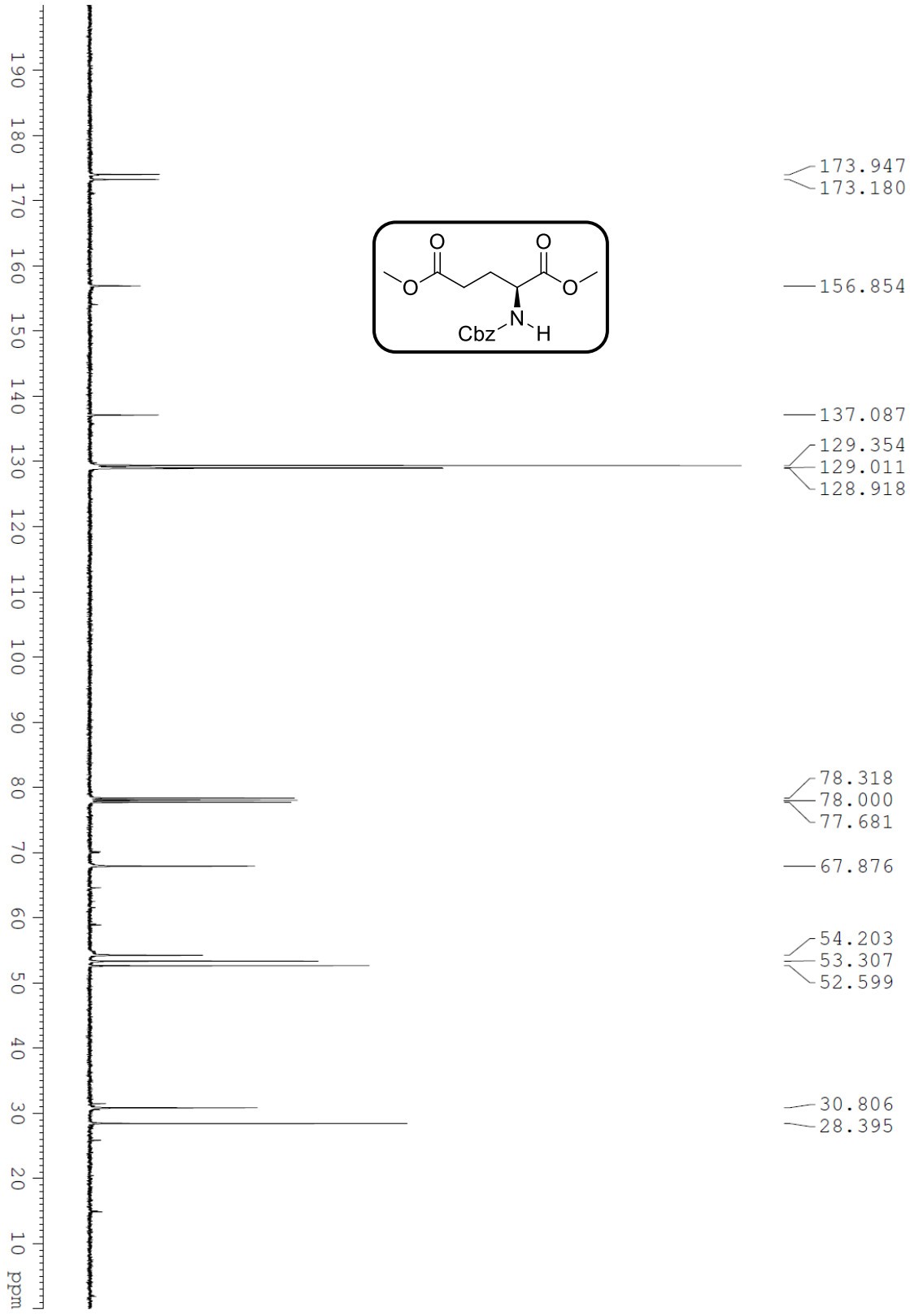
Juan M. López-Soria, Sixto J. Pérez, J. Nicolás Hernández, Miguel A. Ramírez, Víctor S. Martín, and Juan I. Padrón

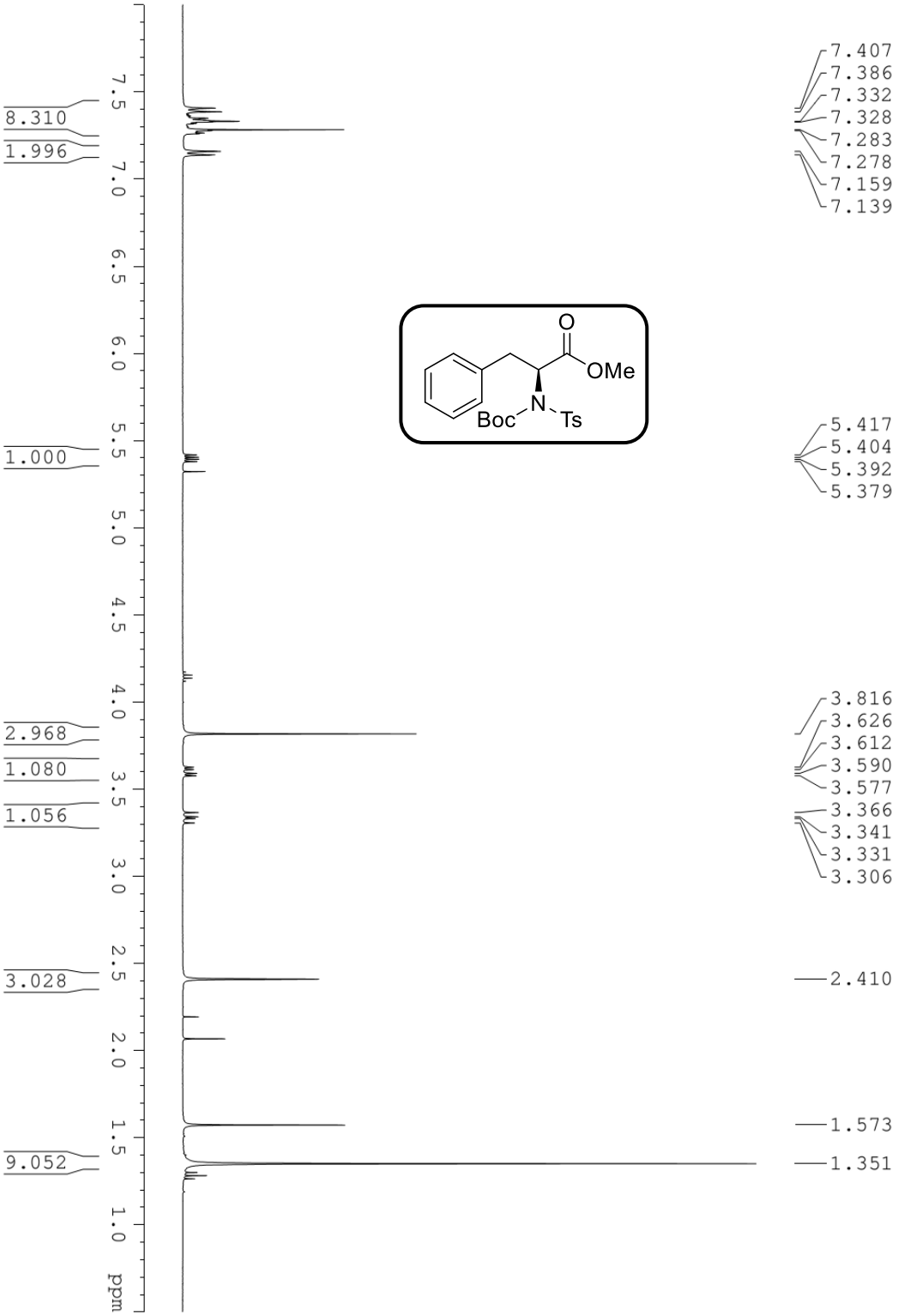

7.393
7.379
7.364
7.358
7.349
7.345
7.339
7.331
7.323
7.310
7.306
7.260
5.241
5.234
5.231
5.024
5.011
5.000
4.987
3.643
3.626
2.537
2.524
2.518
2.504
2.499
2.486
2.482
2.473
2.470
2.465
2.454
2.438
2.415
2.397
2.386
2.379
2.366
2.345
2.341
2.325
2.250
2.235
2.231
2.226
2.216
2.211
5.886
2.000
1.038
5.943
1.185
2.015
1.263
8.936
O
O
O
O
N
Cbz
Boc
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm

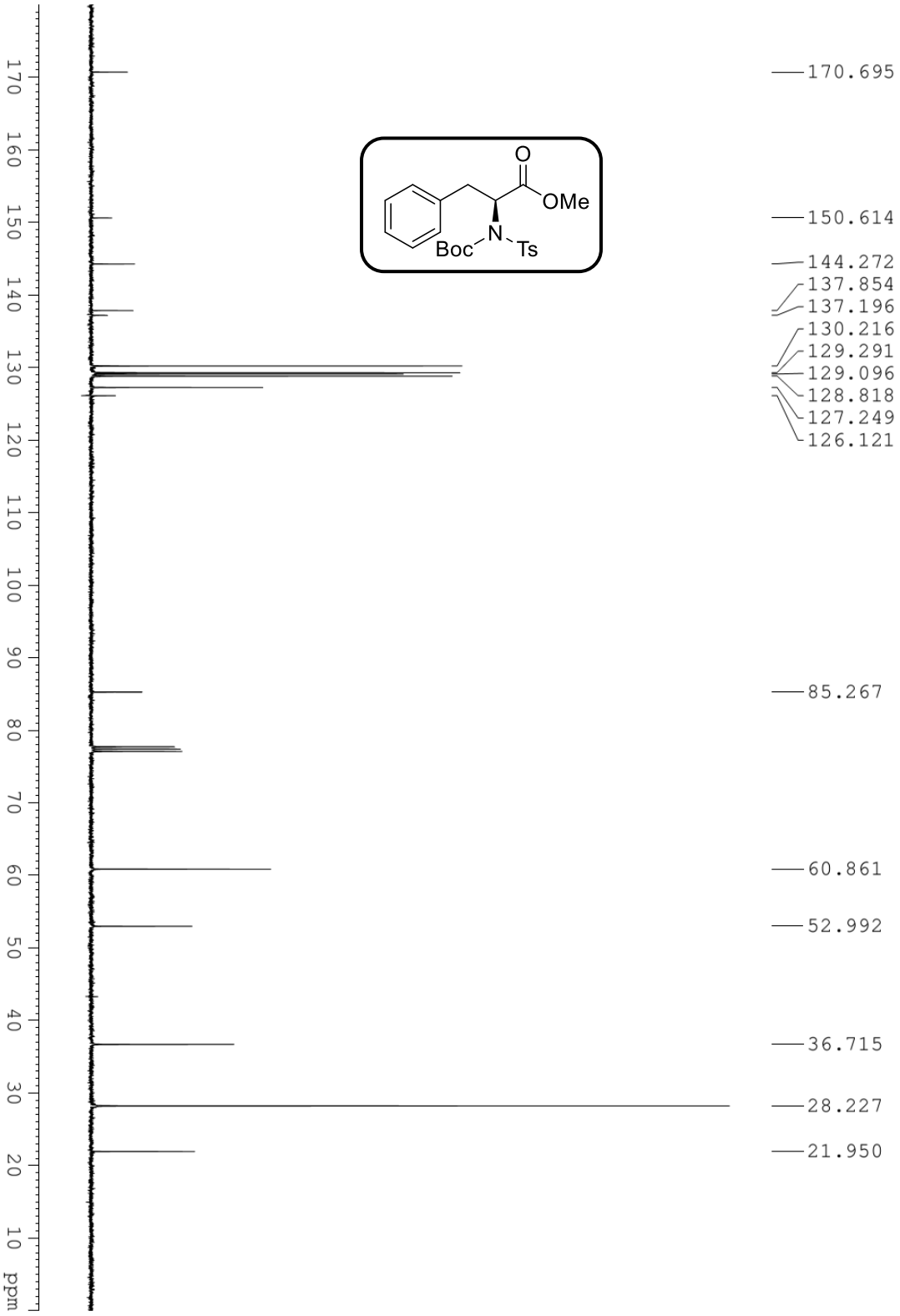


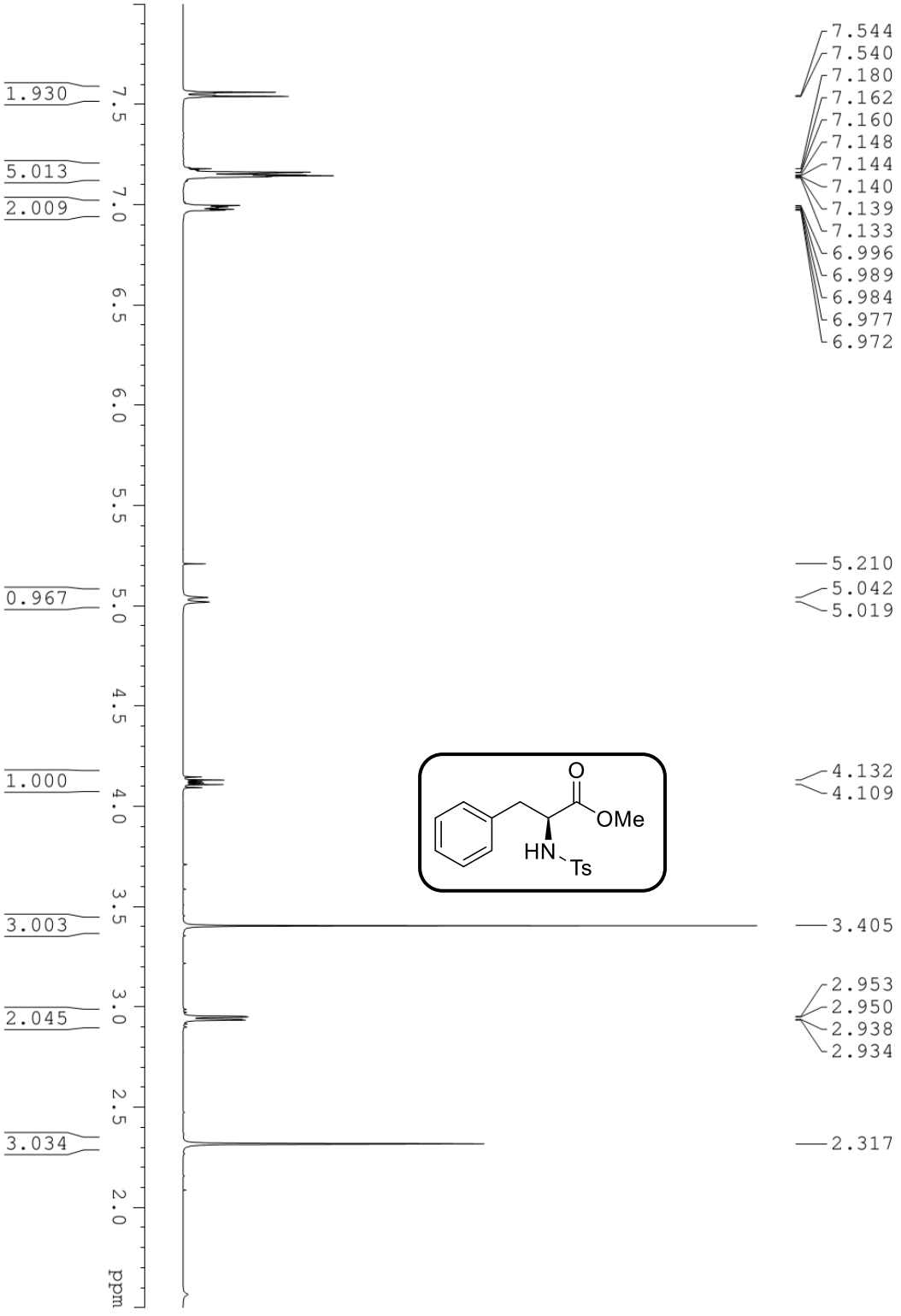
Juan M. López-Soria, Sixto J. Pérez, J. Nicolás Hernández, Miguel A. Ramírez, Víctor S. Martín, and Juan I. Padrón

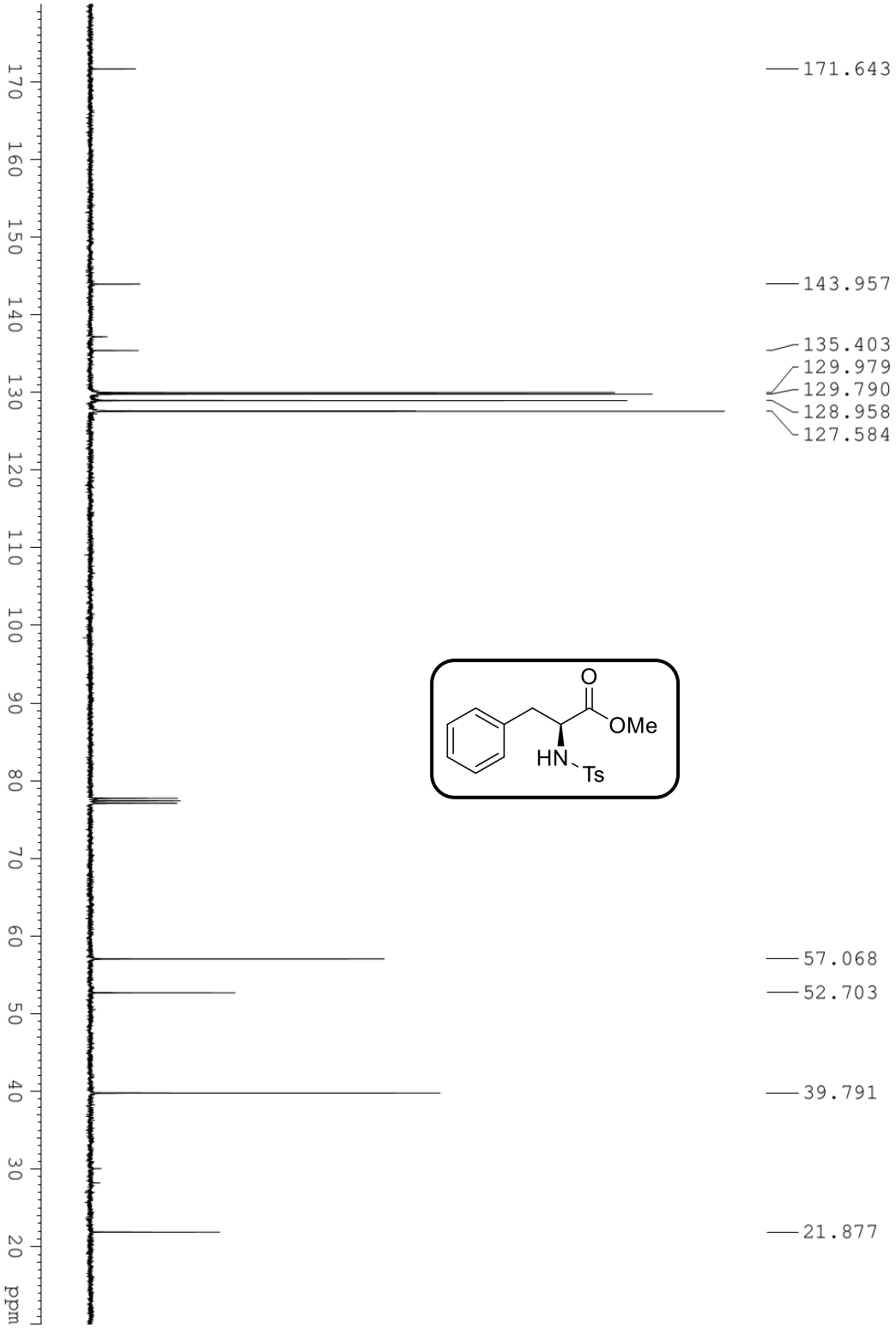

5.402
0.843
2.119
0.979
3.000
3.348
2.197
1.183
1.102
7.353
7.340
7.260
5.390
5.374
5.110
4.428
4.414
3.752
3.661
2.466
2.444
2.424
2.399
2.380
2.356
2.250
2.234
2.216
2.201
2.170
2.040
2.022
2.004
1.986
1.968
O
O
O
O
N
H
Cbz
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm

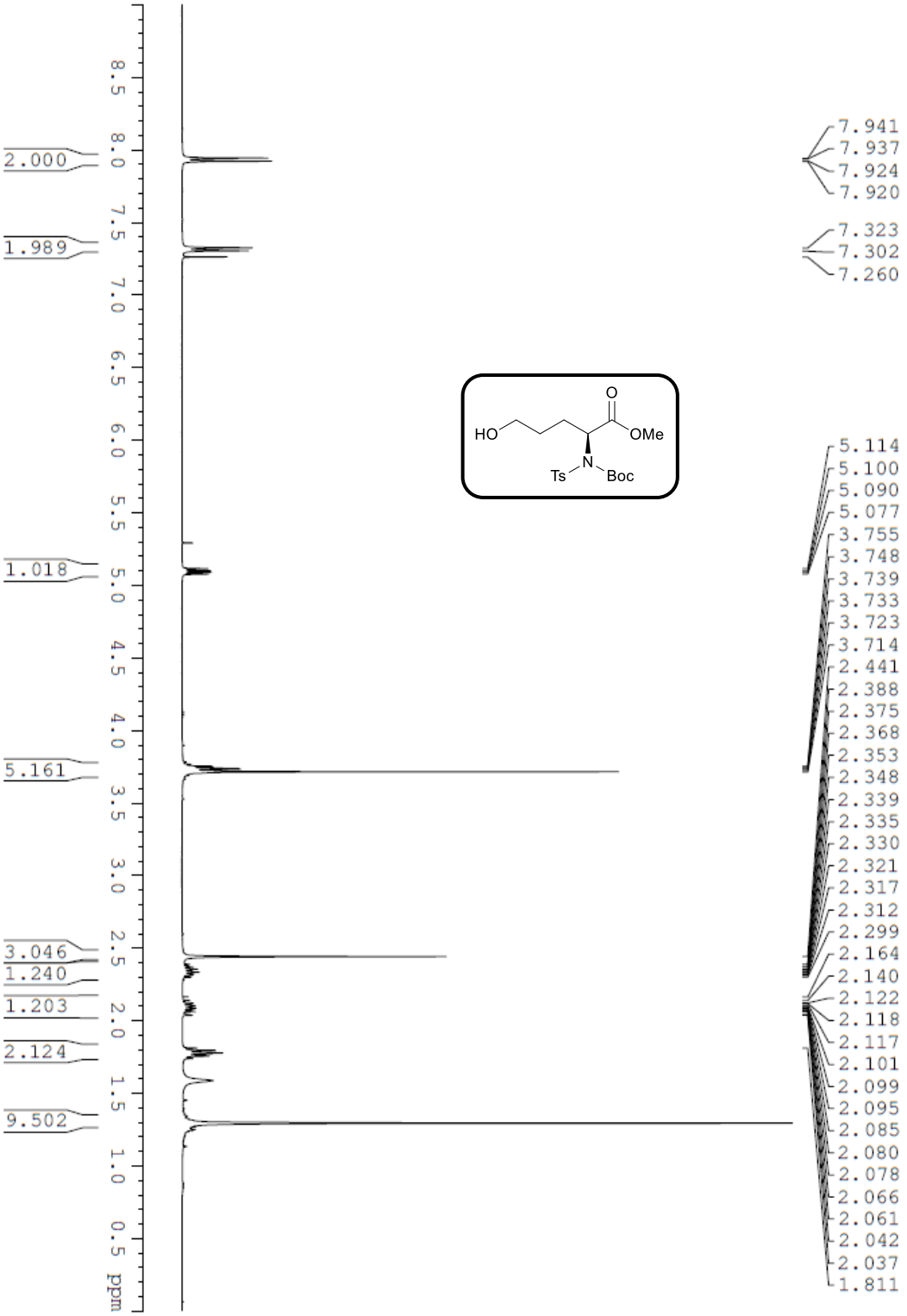

173.947
173.180
156.854
137.087
129.354
129.011
128.918
78.318
78.000
77.681
67.876
54.203
53.307
52.599
30.806
28.395
Cbz
N
H
O
O
O
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

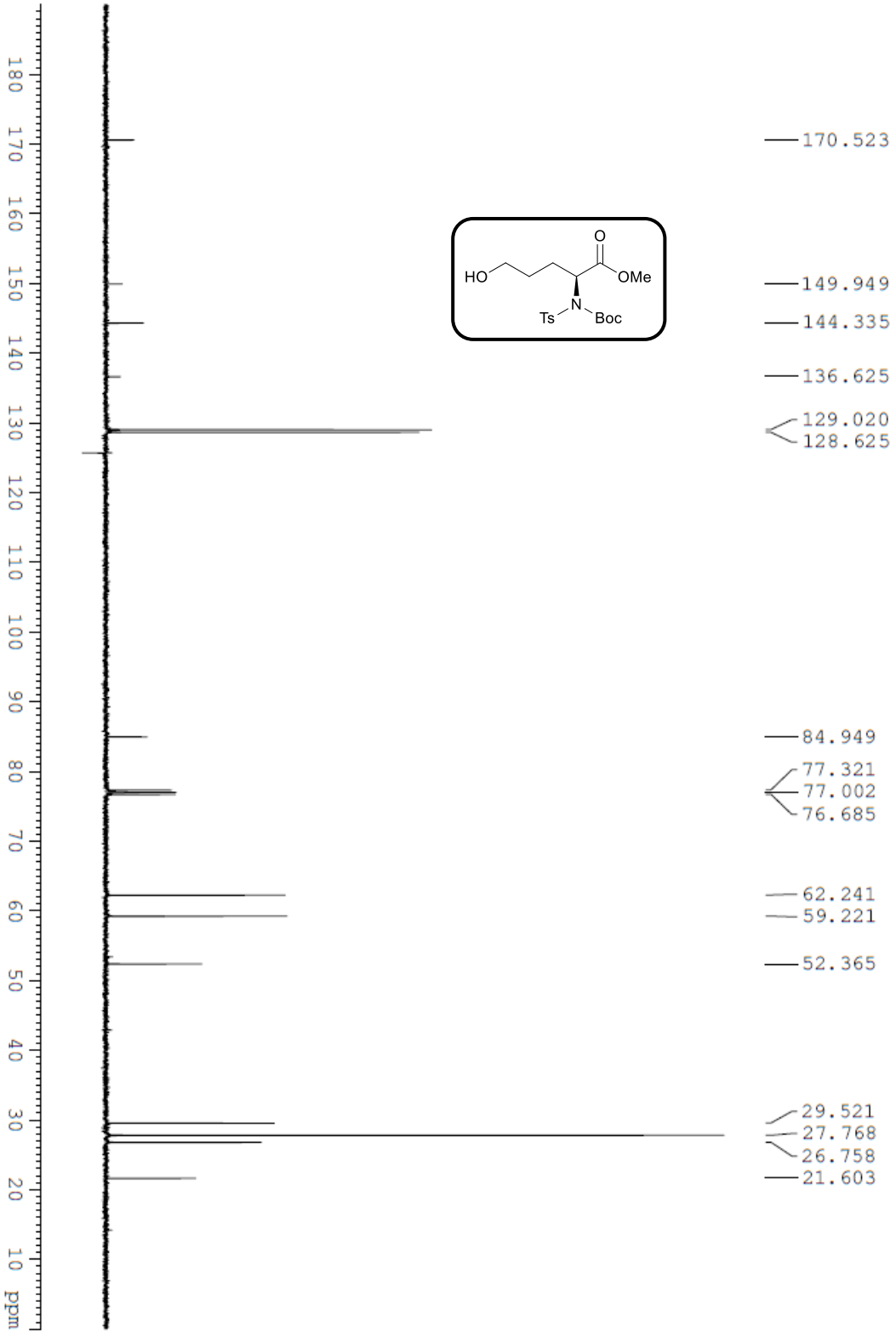

7.407
7.386
7.332
7.328
7.283
7.278
7.159
7.139
8.310
1.996
1.000
5.417
5.404
5.392
5.379
2.968
1.080
1.056
3.816
3.626
3.612
3.590
3.577
3.366
3.341
3.331
3.306
3.028
2.410
1.573
9.052
1.351
O
OMe
N
Boc
Ts
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm

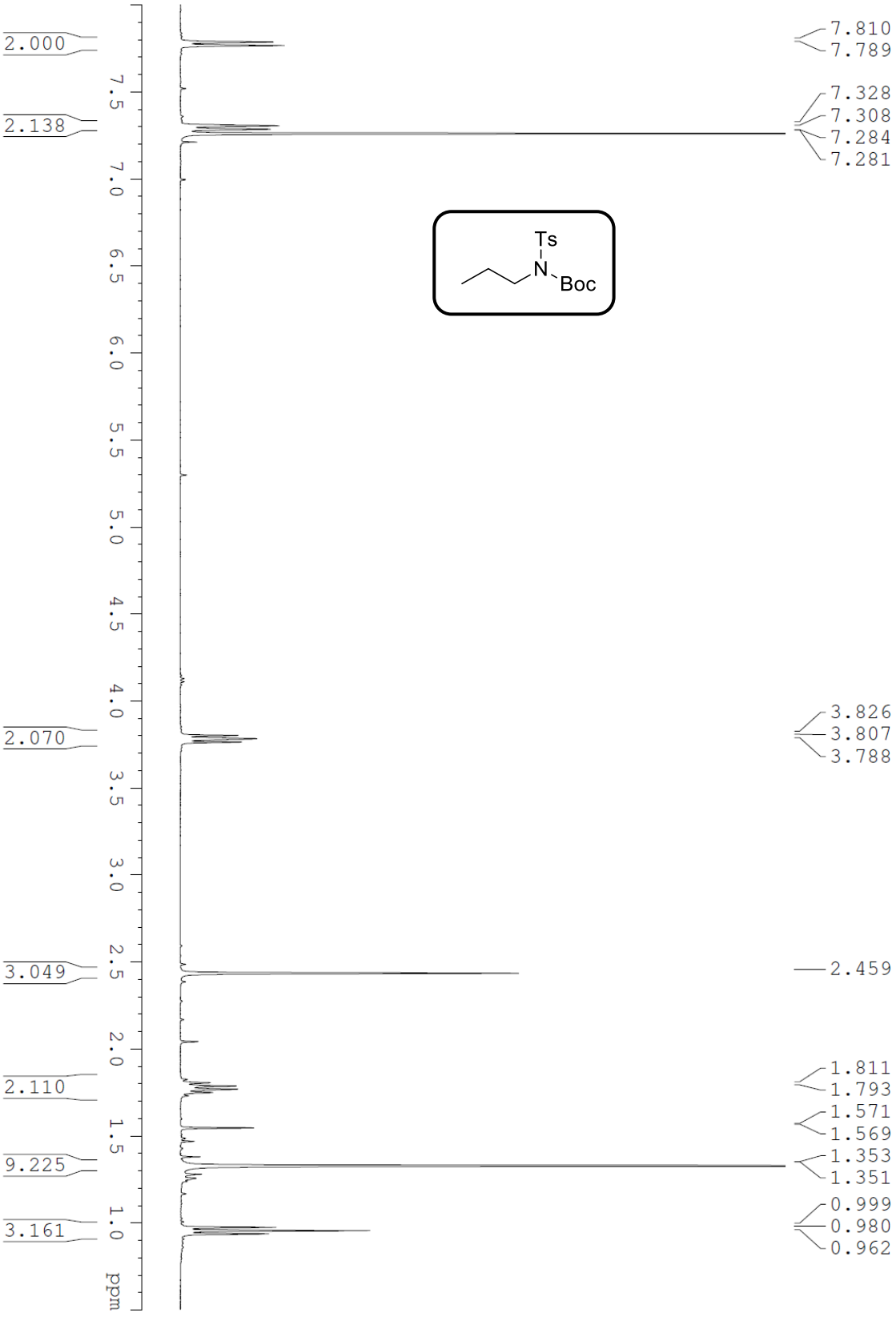

170.695
150.614
144.272
137.854
137.196
130.216
129.291
129.096
128.818
127.249
126.121
85.267
60.861
52.992
36.715
28.227
21.950
O
OMe
N
Boc
Ts
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

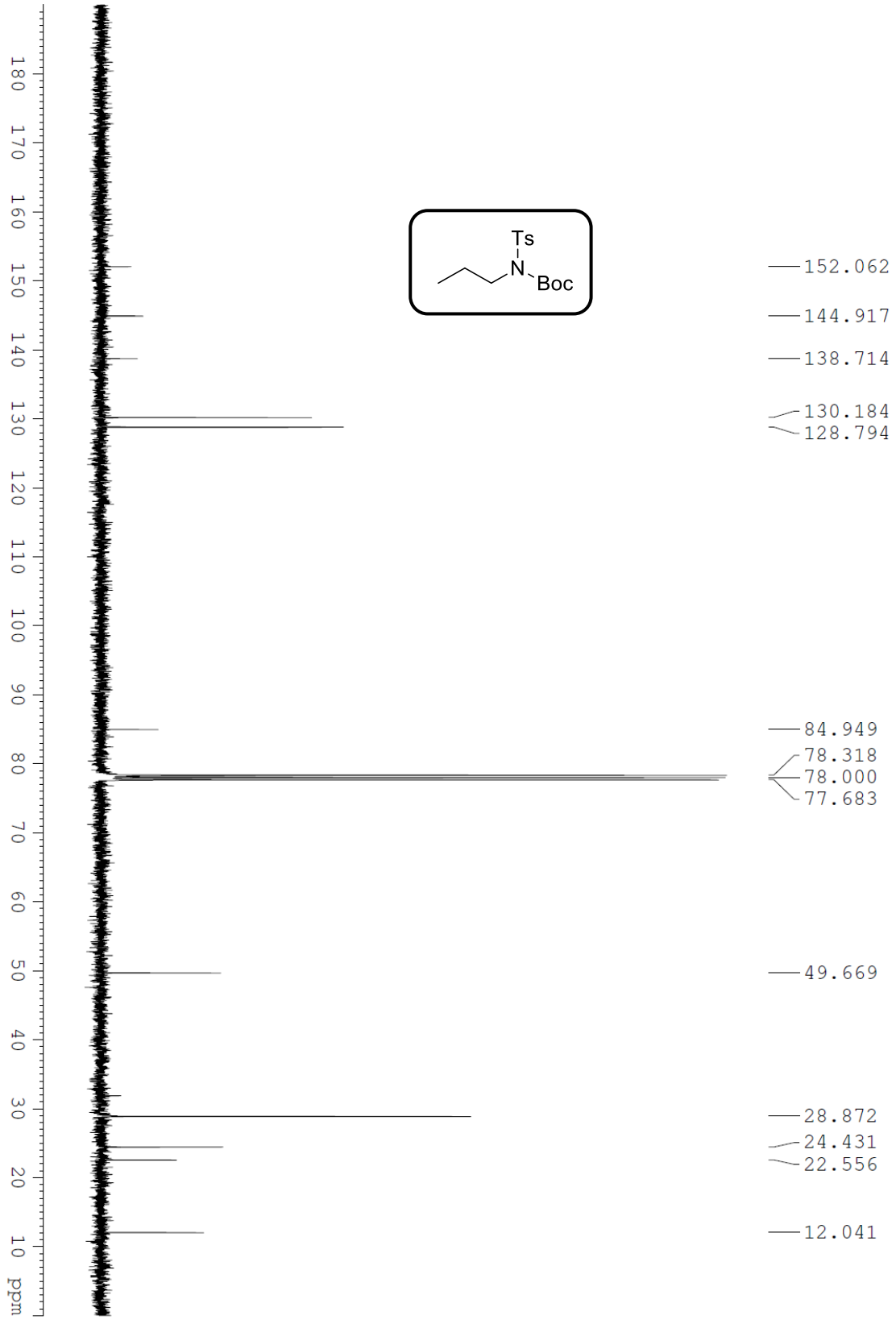

7.544
7.540
7.180
7.162
7.160
7.148
7.144
7.140
7.139
7.133
6.996
6.989
6.984
6.977
6.972
5.210
5.042
5.019
4.132
4.109
3.405
2.953
2.950
2.938
2.934
2.317
1.930
5.013
2.009
0.967
1.000
3.003
2.045
3.034
O
OMe
HN
Ts
ppm

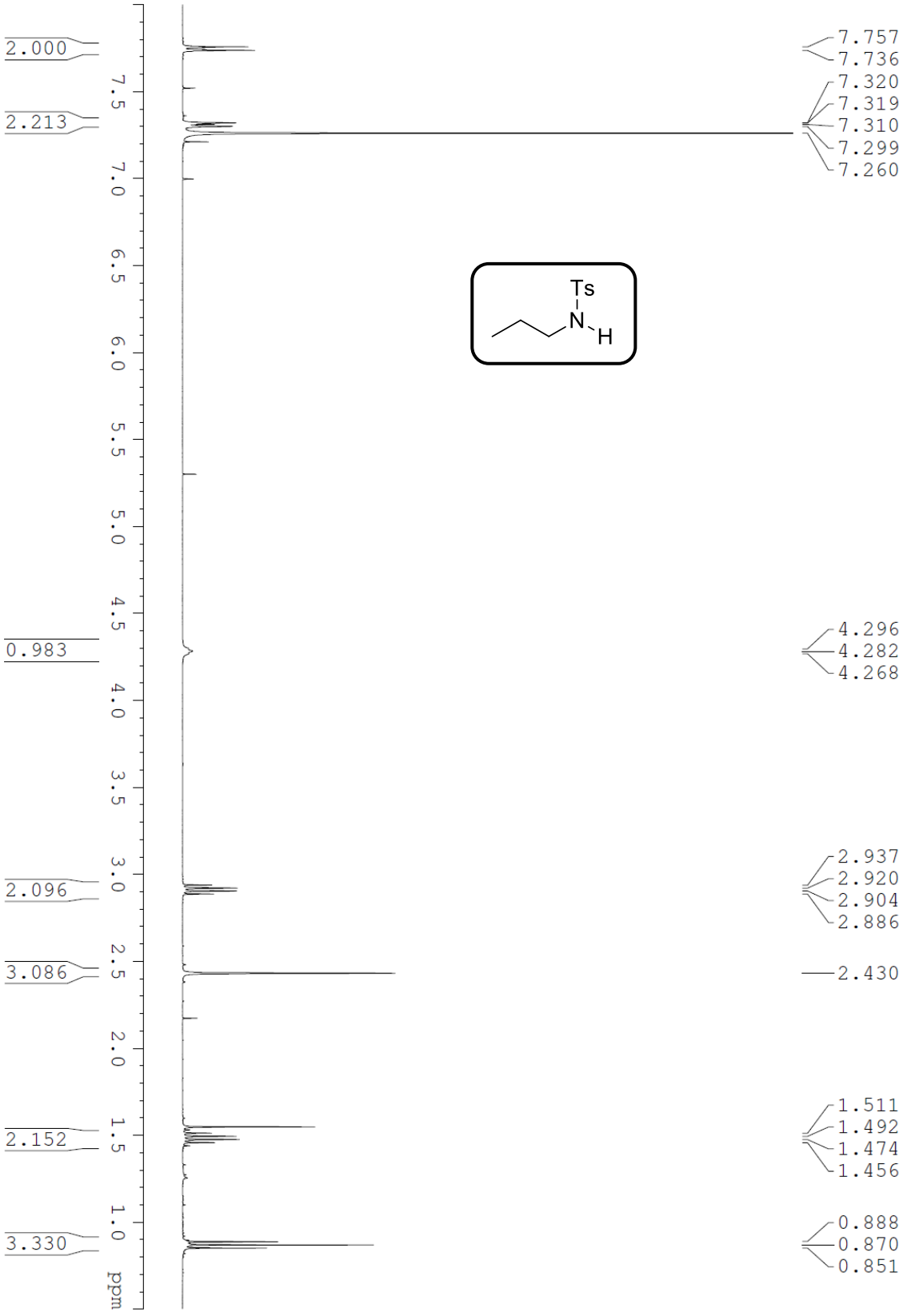

171.643
143.957
135.403
129.979
129.790
128.958
127.584
57.068
52.703
39.791
21.877
O
OMe
HN
Ts
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

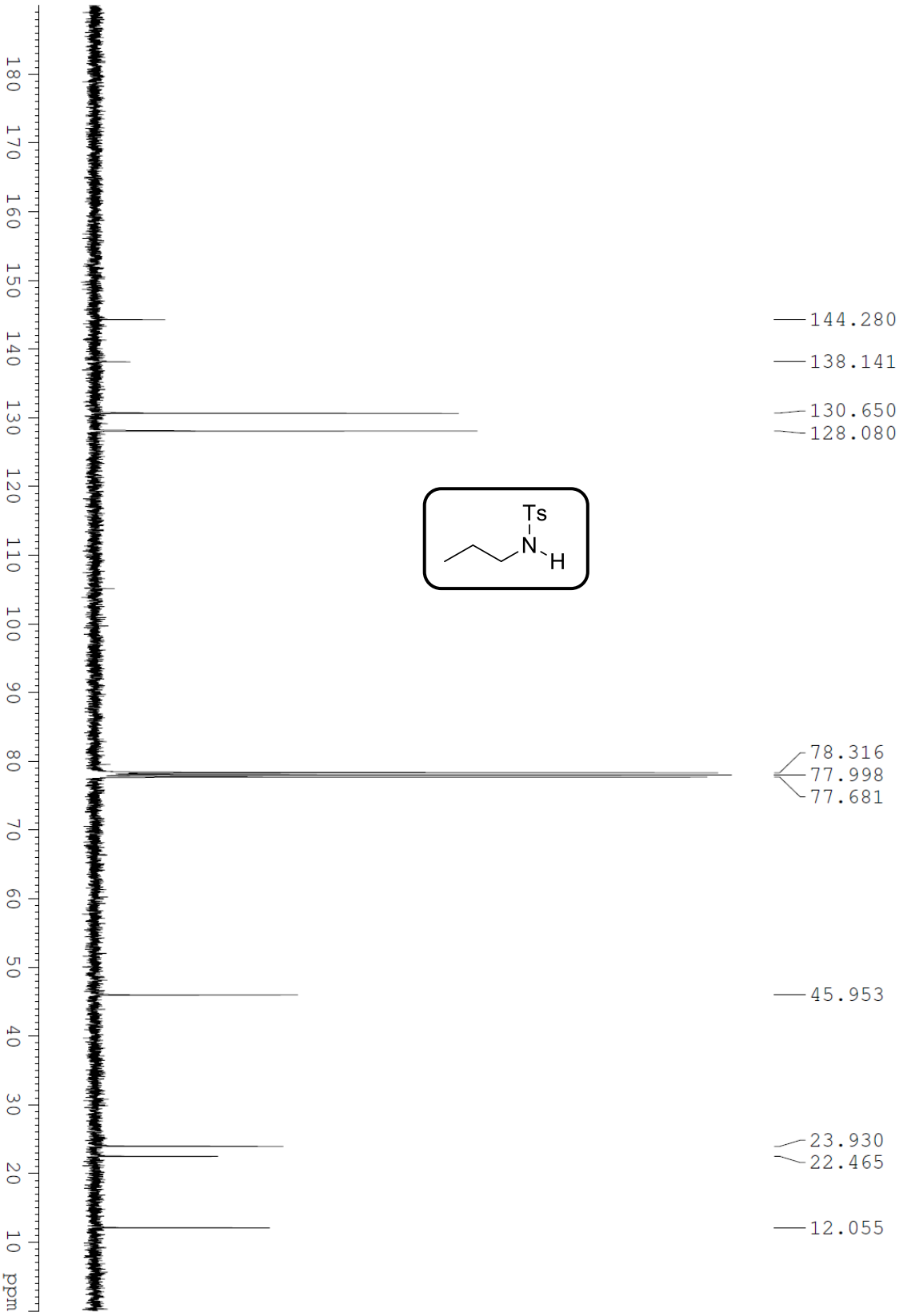

2.000
1.989
1.018
5.161
3.046
1.240
1.203
2.124
9.502
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
7.941
7.937
7.924
7.920
7.323
7.302
7.260
5.114
5.100
5.090
5.077
3.755
3.748
3.739
3.733
3.723
3.714
2.441
2.388
2.375
2.368
2.353
2.348
2.339
2.335
2.330
2.321
2.317
2.312
2.299
2.164
2.140
2.122
2.118
2.117
2.101
2.099
2.095
2.085
2.080
2.078
2.066
2.061
2.042
2.037
1.811
HO
O
OMe
N
Ts
Boc

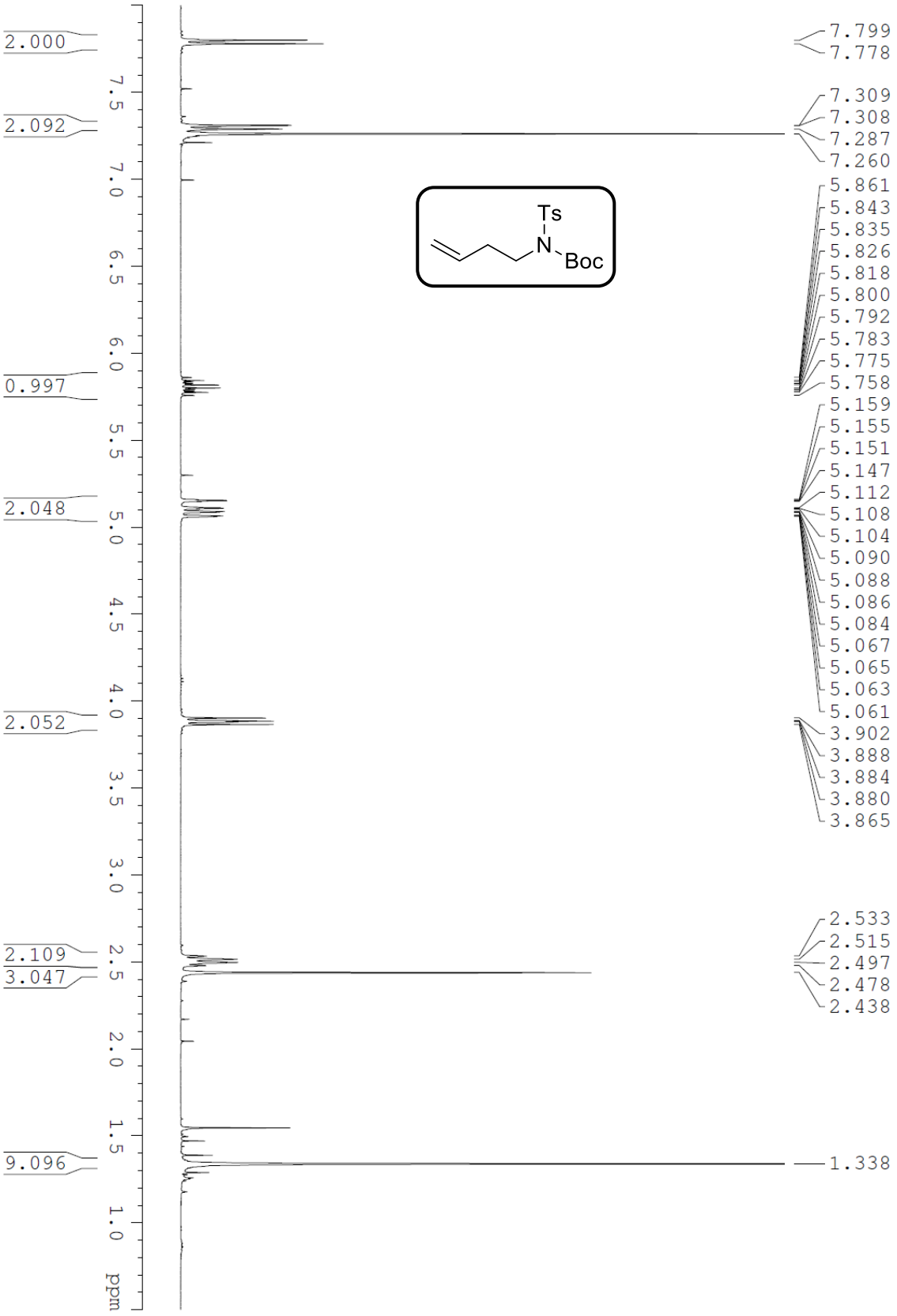

170.523
149.949
144.335
136.625
129.020
128.625
84.949
77.321
77.002
76.685
62.241
59.221
52.365
29.521
27.768
26.758
21.603
HO
O
OMe
N
Ts
Boc
ppm

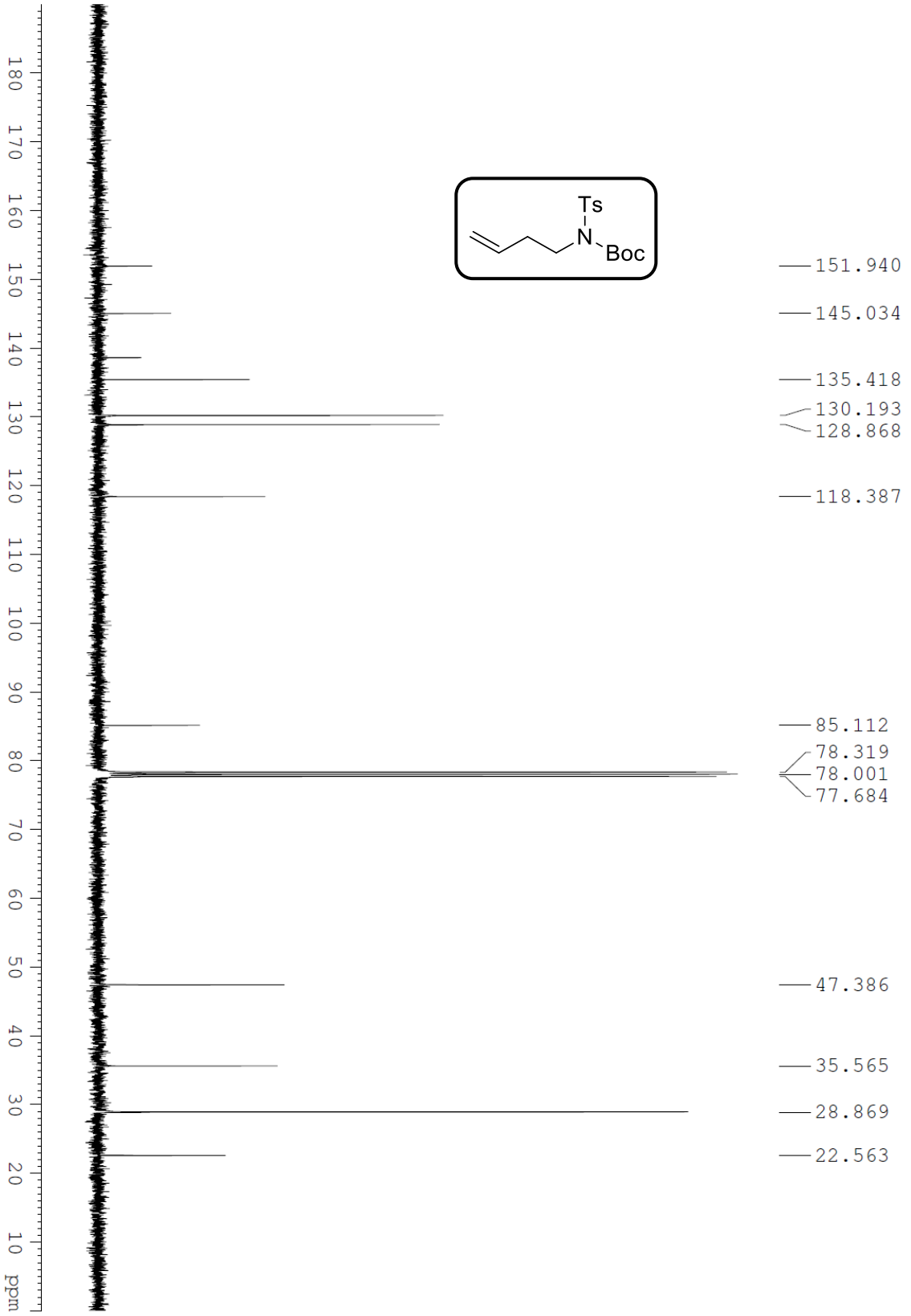

2.000
2.138
2.070
3.049
2.110
9.225
3.161
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
7.810
7.789
7.328
7.308
7.284
7.281
Ts
N
Boc
3.826
3.807
3.788
2.459
1.811
1.793
1.571
1.569
1.353
1.351
0.999
0.980
0.962

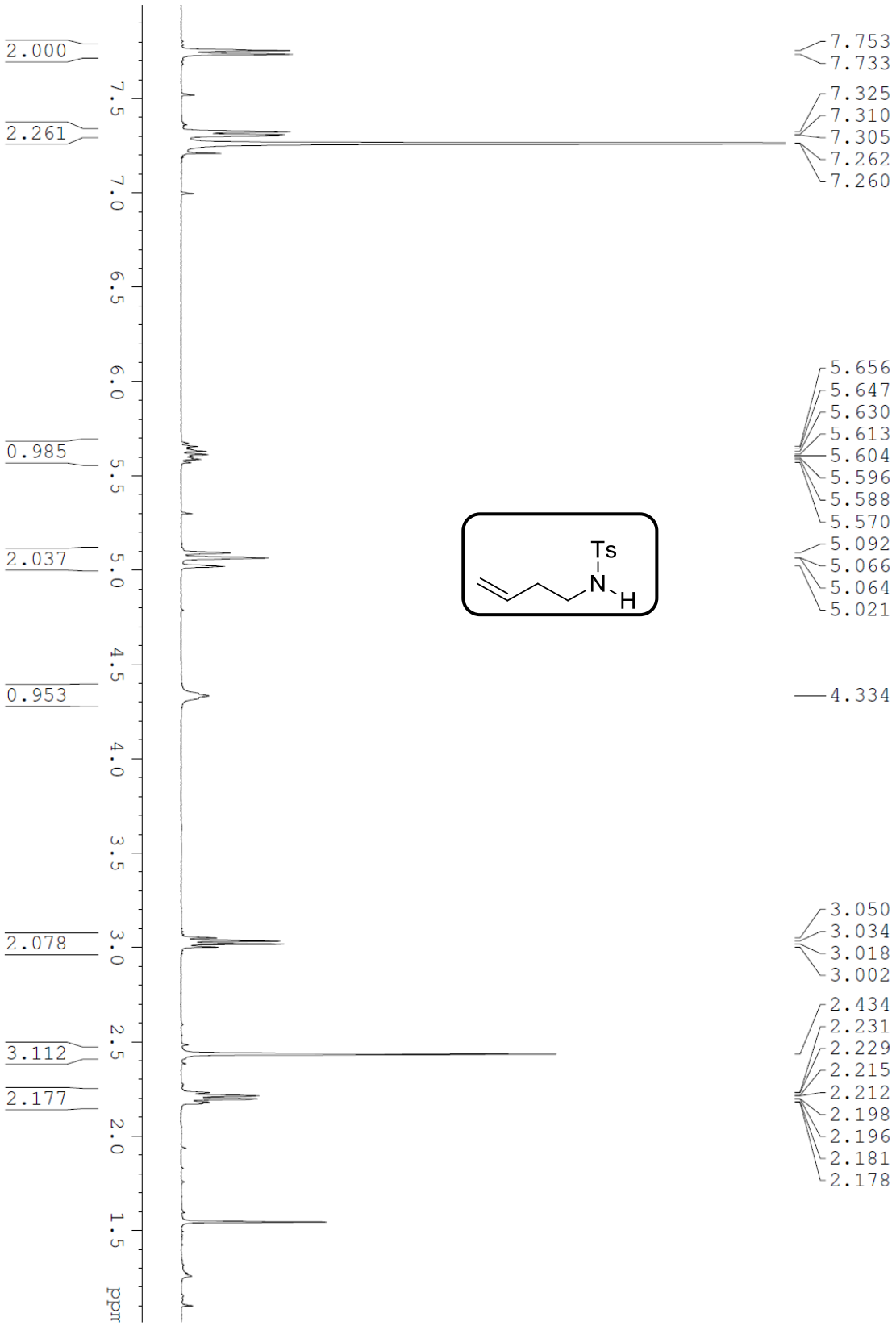

Ts
N
Boc
152.062
144.917
138.714
130.184
128.794
84.949
78.318
78.000
77.683
49.669
28.872
24.431
22.556
12.041
ppm

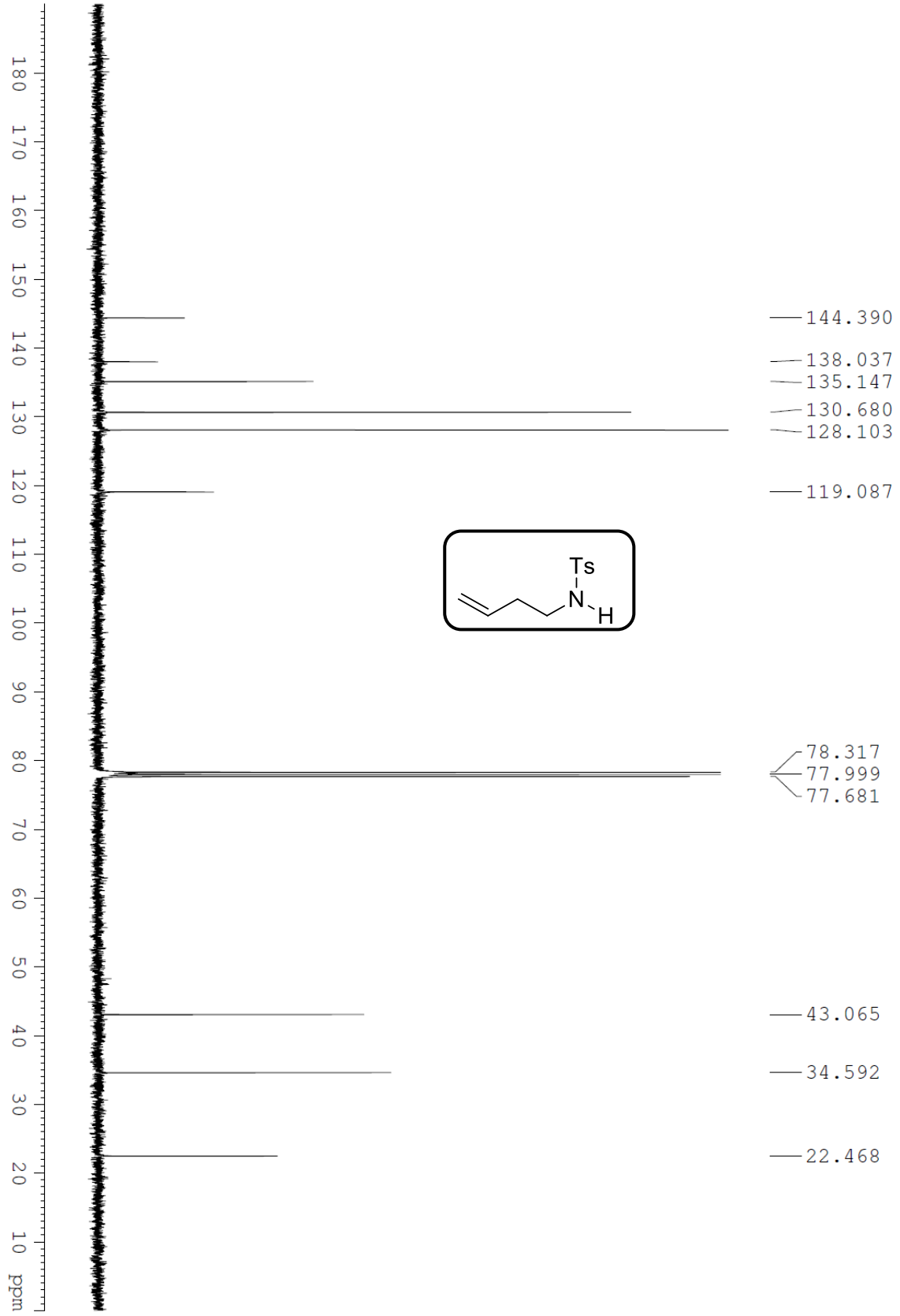

2.000
2.213
0.983
2.096
3.086
2.152
3.330
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
7.757
7.736
7.320
7.319
7.310
7.299
7.260
Ts
N
H
4.296
4.282
4.268
2.937
2.920
2.904
2.886
2.430
1.511
1.492
1.474
1.456
0.888
0.870
0.851

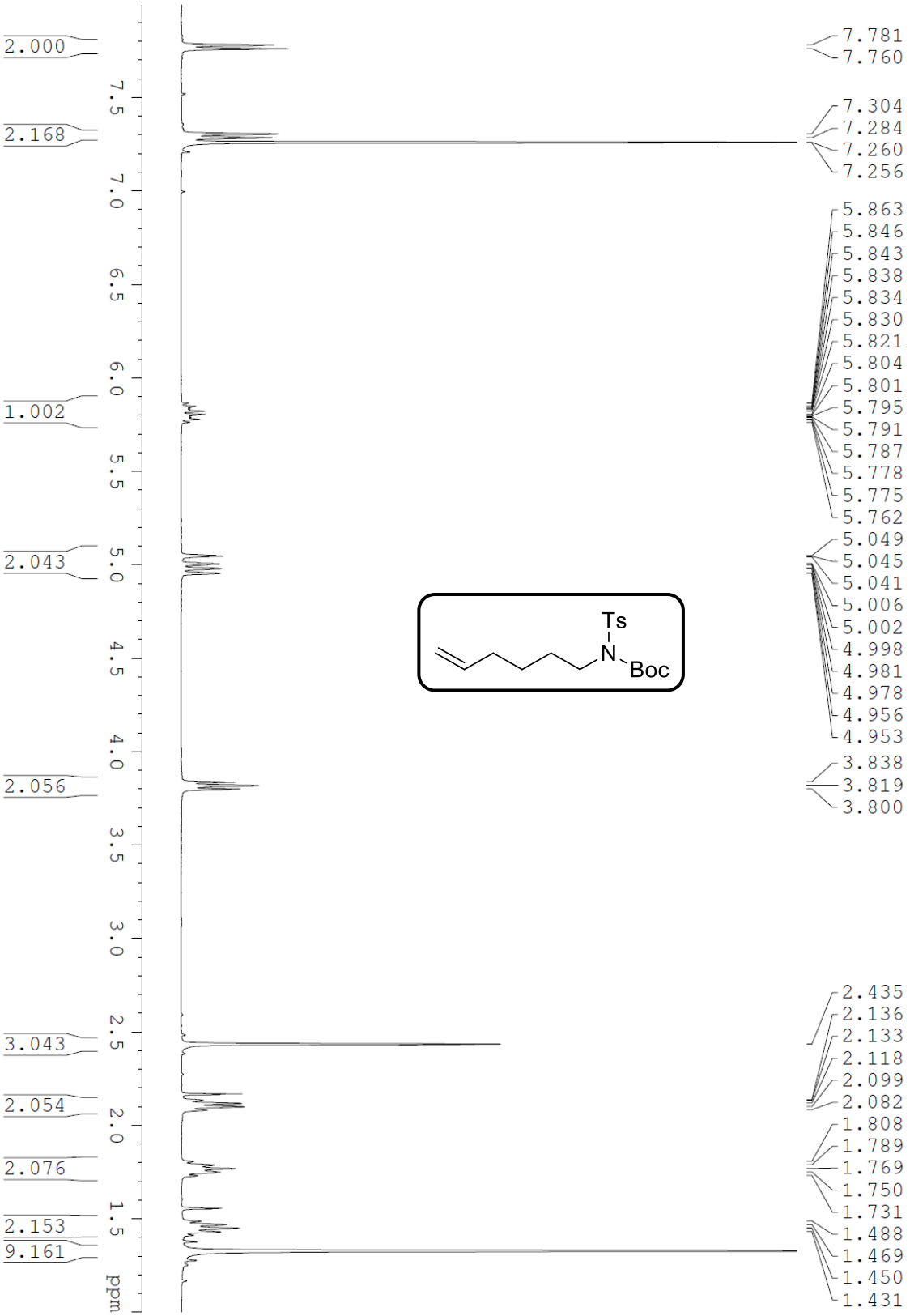

144.280
138.141
130.650
128.080
Ts
N
H
78.316
77.998
77.681
45.953
23.930
22.465
12.055
ppm

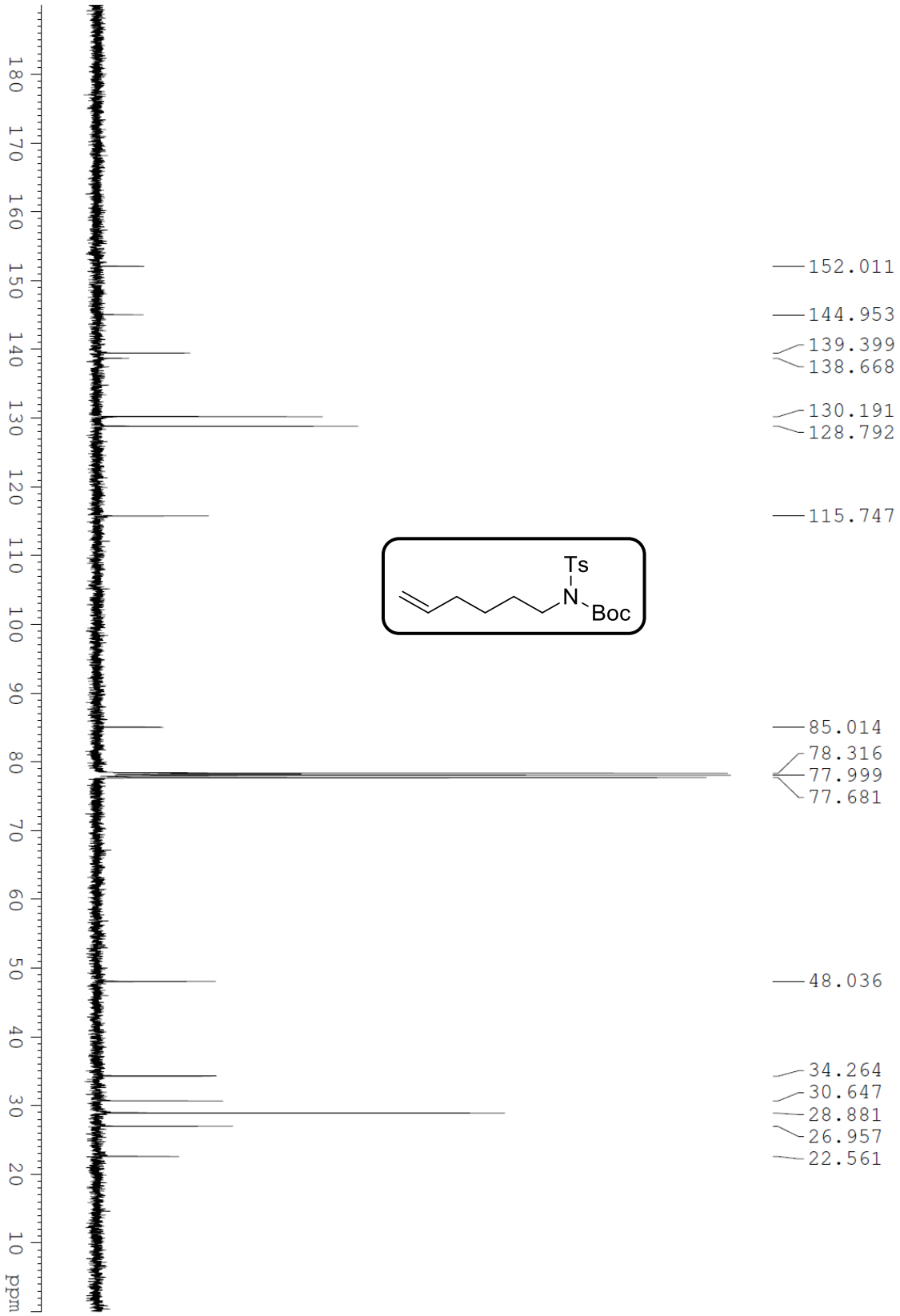

2.000
2.092
0.997
2.048
2.052
2.109
3.047
9.096
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
Ts
N
Boc
7.799
7.778
7.309
7.308
7.287
7.260
5.861
5.843
5.835
5.826
5.818
5.800
5.792
5.783
5.775
5.758
5.159
5.155
5.151
5.147
5.112
5.108
5.104
5.090
5.088
5.086
5.084
5.067
5.065
5.063
5.061
3.902
3.888
3.884
3.880
3.865
2.533
2.515
2.497
2.478
2.438
1.338

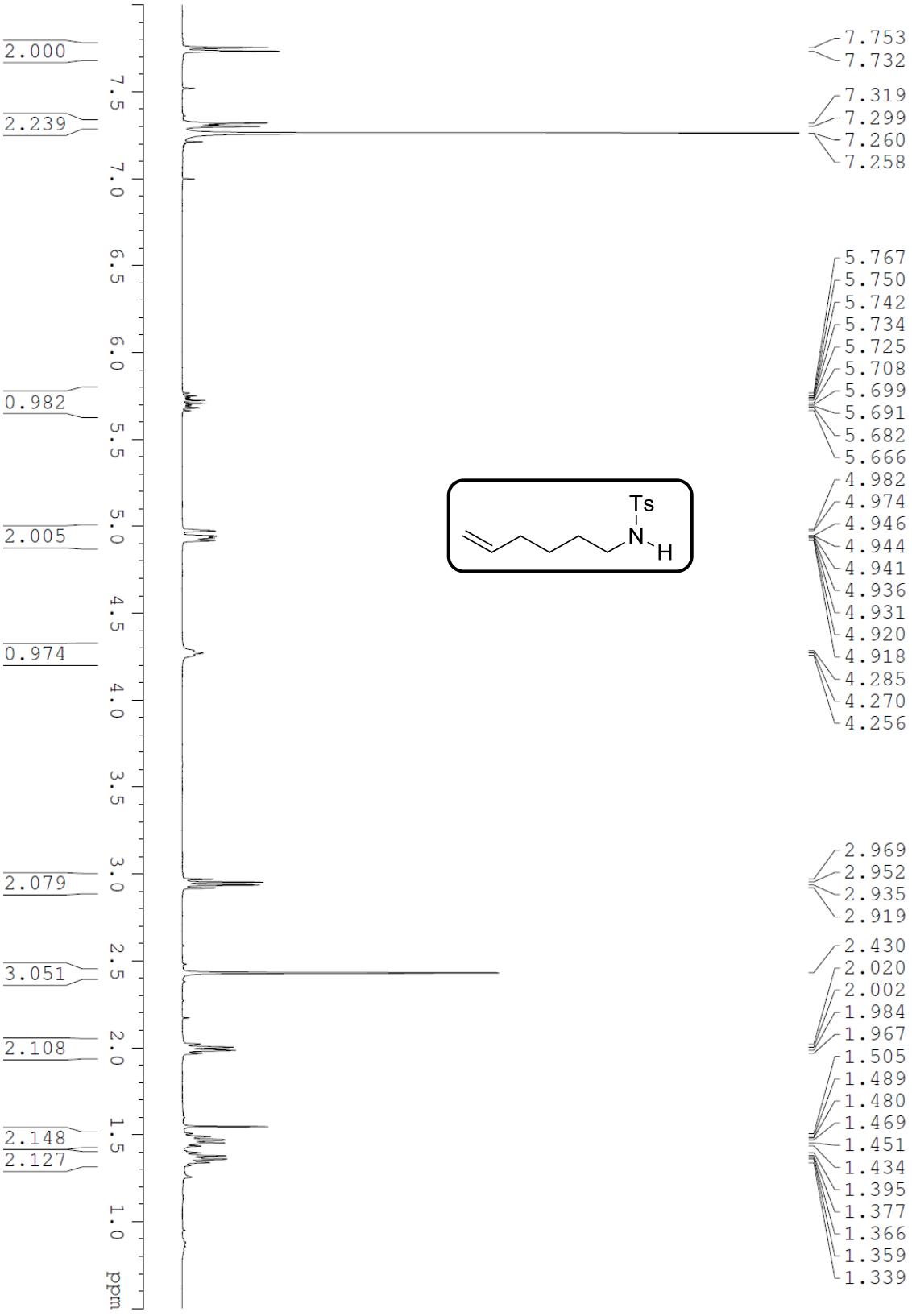

Ts
N
Boc
151.940
145.034
135.418
130.193
128.868
118.387
85.112
78.319
78.001
77.684
47.386
35.565
28.869
22.563
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

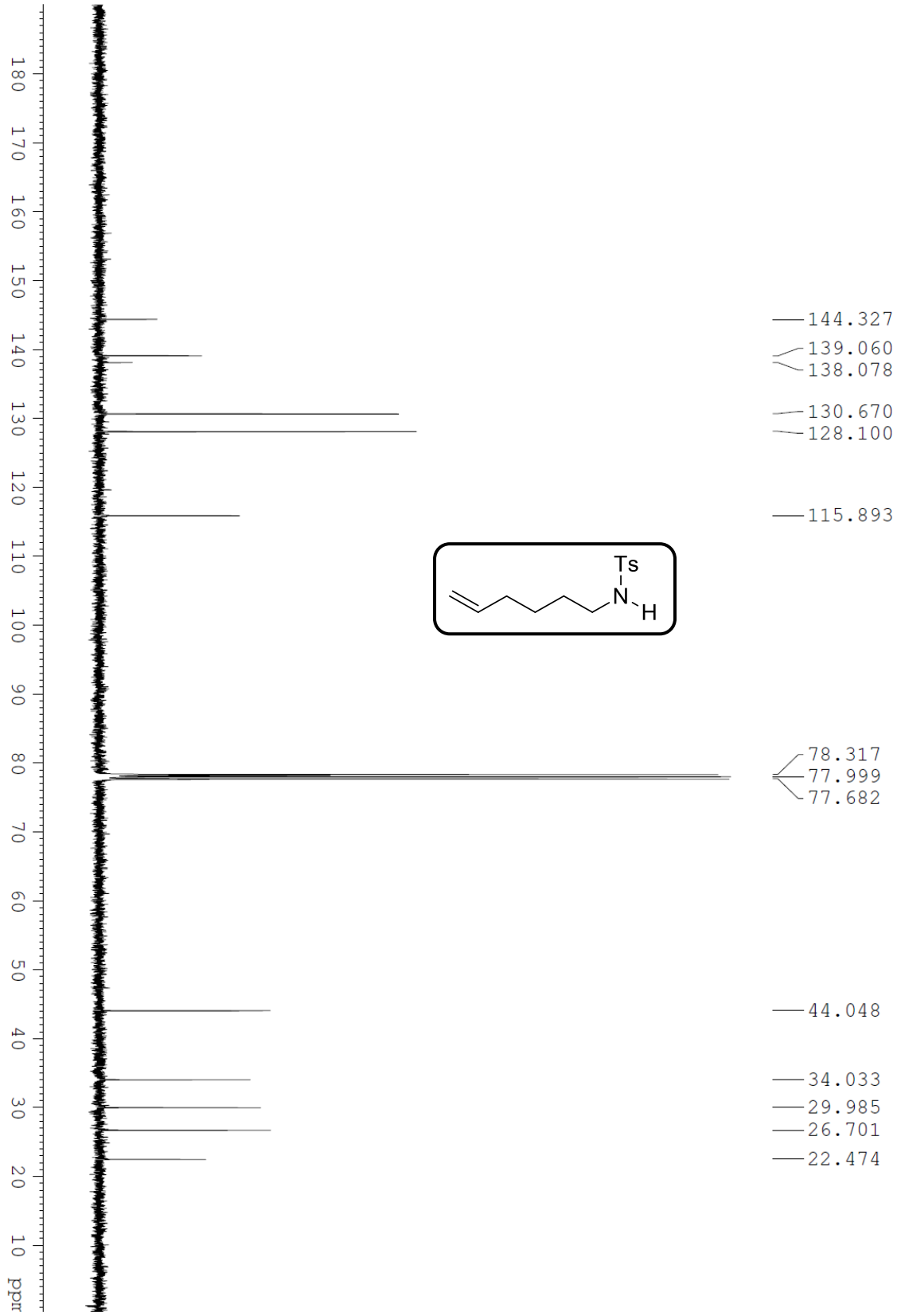

2.000
2.261
0.985
2.037
0.953
2.078
3.112
2.177
7.753
7.733
7.325
7.310
7.305
7.262
7.260
5.656
5.647
5.630
5.613
5.604
5.596
5.588
5.570
5.092
5.066
5.064
5.021
4.334
3.050
3.034
3.018
3.002
2.434
2.231
2.229
2.215
2.212
2.198
2.196
2.181
2.178
Ts
N
H
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm


144.390
138.037
135.147
130.680
128.103
119.087
Ts
N
H
78.317
77.999
77.681
43.065
34.592
22.468
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


2.000
2.168
1.002
2.043
2.056
3.043
2.054
2.076
2.153
9.161
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
7.781
7.760
7.304
7.284
7.260
7.256
5.863
5.846
5.843
5.838
5.834
5.830
5.821
5.804
5.801
5.795
5.791
5.787
5.778
5.775
5.762
5.049
5.045
5.041
5.006
5.002
4.998
4.981
4.978
4.956
4.953
3.838
3.819
3.800
2.435
2.136
2.133
2.118
2.099
2.082
1.808
1.789
1.769
1.750
1.731
1.488
1.469
1.450
1.431
Ts
N
Boc


180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
152.011
144.953
139.399
138.668
130.191
128.792
115.747
85.014
78.316
77.999
77.681
48.036
34.264
30.647
28.881
26.957
22.561
Ts
N
Boc


2.000
2.239
0.982
2.005
0.974
2.079
3.051
2.108
2.148
2.127
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
7.753
7.732
7.319
7.299
7.260
7.258
5.767
5.750
5.742
5.734
5.725
5.708
5.699
5.691
5.682
5.666
4.982
4.974
4.946
4.944
4.941
4.936
4.931
4.920
4.918
4.285
4.270
4.256
2.969
2.952
2.935
2.919
2.430
2.020
2.002
1.984
1.967
1.505
1.489
1.480
1.469
1.451
1.434
1.395
1.377
1.366
1.359
1.339
Ts
N
H


144.327
139.060
138.078
130.670
128.100
115.893
78.317
77.999
77.682
44.048
34.033
29.985
26.701
22.474
Ts
N
H
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

OPTIMIZED STRUCTURES (B3LYP/Def2-SVP, solvent=CH_2Cl_2) IN MOL FORMAT REFERENCED IN TABLE 4.

Entry 1A **Lewis acid = null**

Title Card Required

Created by GaussView 5.0.9

```
 28 27  0  0  0  0  0  0  0  0  0    0
   -1.0942    0.9159   -0.1541 N   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9050    2.1393   -0.1513 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9147    1.8992   -0.4987 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9640    2.5859    0.8537 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4413    2.8630   -0.8330 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.2956    1.0596   -0.1017 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.8266    2.1442   -0.0005 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.9039   -0.1197   -0.2227 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.3536   -0.3018    0.0130 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.5249   -1.8155   -0.1102 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.5725   -2.0923    0.0799 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.8849   -2.3349    0.6182 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.2561   -2.1590   -1.1208 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.7038    0.1742    1.4244 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.5751    1.2596    1.5256 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.0680   -0.3312    2.1673 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.7534   -0.0739    1.6436 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.1458    0.4335   -1.0694 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.8287    0.1022   -2.0704 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.0087    1.5196   -0.9946 H   0  0  0  0  0  0  0  0  0  0  0  0
    4.2168    0.2044   -0.9578 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8803   -0.5935    0.1677 S   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2331   -1.2530    1.3019 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.3071   -0.2666    0.2494 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6058   -1.5526   -1.3186 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0652   -1.0173   -2.1585 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5278   -1.6855   -1.4567 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1070   -2.5147   -1.1455 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  6  1  0  0  0  0
  1 22  1  0  0  0  0
  2  3  1  0  0  0  0
  2  4  1  0  0  0  0
  2  5  1  0  0  0  0
  6  7  2  0  0  0  0
  6  8  4  0  0  0  0
  8  9  1  0  0  0  0
  9 10  1  0  0  0  0
  9 14  1  0  0  0  0
```

```
 9 18  1  0  0  0  0
10 11  1  0  0  0  0
10 12  1  0  0  0  0
10 13  1  0  0  0  0
14 15  1  0  0  0  0
14 16  1  0  0  0  0
14 17  1  0  0  0  0
18 19  1  0  0  0  0
18 20  1  0  0  0  0
18 21  1  0  0  0  0
22 23  2  0  0  0  0
22 24  2  0  0  0  0
22 25  1  0  0  0  0
25 26  1  0  0  0  0
25 27  1  0  0  0  0
25 28  1  0  0  0  0
```

Entry 1B **Lewis acid = null**

Title Card Required

```
Created by GaussView 5.0.9
 25 24  0  0  0  0  0  0  0  0  0    0
    1.9524    0.1952    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    3.1524   -0.6212    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.7676   -0.4115   -0.8929 H   0  0  0  0  0  0  0  0  0  0  0  0
    3.7680   -0.4108    0.8926 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.8709   -1.6796    0.0005 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.7271   -0.4146    0.0001 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.5713   -1.6276   -0.0001 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.2783    0.4859    0.0003 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6900    0.0878    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4231    1.4311    0.0001 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.5115    1.2696    0.0001 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1591    2.0182    0.8931 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1590    2.0184   -0.8926 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0151   -0.7018    1.2720 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4819   -1.6602    1.2884 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7318   -0.1220    2.1646 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.0978   -0.8961    1.3209 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0148   -0.7013   -1.2724 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7311   -0.1213   -2.1647 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.4817   -1.6599   -1.2889 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.0975   -0.8955   -1.3217 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.1585    1.6330   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.1989    2.1570   -0.0007 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.7324    1.9418    0.8920 H   0  0  0  0  0  0  0  0  0  0  0  0
```

```
   2.7334    1.9414   -0.8915 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  6  4  0  0  0  0
 1 22  1  0  0  0  0
 2  3  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 6  7  2  0  0  0  0
 6  8  1  0  0  0  0
 8  9  1  0  0  0  0
 9 10  1  0  0  0  0
 9 14  1  0  0  0  0
 9 18  1  0  0  0  0
10 11  1  0  0  0  0
10 12  1  0  0  0  0
10 13  1  0  0  0  0
14 15  1  0  0  0  0
14 16  1  0  0  0  0
14 17  1  0  0  0  0
18 19  1  0  0  0  0
18 20  1  0  0  0  0
18 21  1  0  0  0  0
22 23  1  0  0  0  0
22 24  1  0  0  0  0
22 25  1  0  0  0  0
```

Entry 2A **Lewis acid = H+**

Title Card Required

Created by GaussView 5.0.9

```
 29 26  0  0  0  0  0  0  0  0  0  0    0
   -1.0790    0.9561   -0.1135 N   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9144    2.1657   -0.0246 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9588    1.8663   -0.1543 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7925    2.6452    0.9565 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6252    2.8636   -0.8203 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.2438    1.0404   -0.2075 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.7635    2.2318   -0.0902 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.9214   -0.0230   -0.4460 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.3455   -0.3650    0.0540 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.4402   -1.8377   -0.3115 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.4076   -2.2309    0.0327 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.6348   -2.4056    0.1741 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.3766   -1.9774   -1.4004 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.3595   -0.1322    1.5578 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.2406    0.9301    1.8189 H   0  0  0  0  0  0  0  0  0  0  0  0
```

```
   1.5671   -0.7150    2.0476 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.3319   -0.4615    1.9530 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.3493    0.4810   -0.7191 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.1563    0.4445   -1.8006 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.3924    1.5306   -0.3822 H   0  0  0  0  0  0  0  0  0  0  0  0
   4.3556    0.0738   -0.5405 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.8602   -0.6639    0.1634 S   0  0  0  0  0  0  0  0  0  0  0  0
  -1.0283   -1.3687    1.1274 O   0  0  0  0  0  0  0  0  0  0  0  0
  -3.2397   -0.3148    0.4665 O   0  0  0  0  0  0  0  0  0  0  0  0
  -1.7530   -1.4171   -1.4503 C   0  0  0  0  0  0  0  0  0  0  0  0
  -2.3162   -0.7929   -2.1545 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.6962   -1.5113   -1.7240 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.2225   -2.4045   -1.3368 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.7038    2.2618   -0.3447 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  6  4  0  0  0  0
 2  3  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 6  7  4  0  0  0  0
 6  8  2  0  0  0  0
 7 29  1  0  0  0  0
 9 10  1  0  0  0  0
 9 14  1  0  0  0  0
 9 18  1  0  0  0  0
10 11  1  0  0  0  0
10 12  1  0  0  0  0
10 13  1  0  0  0  0
14 15  1  0  0  0  0
14 16  1  0  0  0  0
14 17  1  0  0  0  0
18 19  1  0  0  0  0
18 20  1  0  0  0  0
18 21  1  0  0  0  0
22 23  2  0  0  0  0
22 24  2  0  0  0  0
22 25  1  0  0  0  0
25 26  1  0  0  0  0
25 27  1  0  0  0  0
25 28  1  0  0  0  0
```

Entry 2B **Lewis acid = H+**

itle Card Required

Created by GaussView 5.0.9

```
 26 24  0  0  0  0  0  0  0  0  0    0
```

1.9403	0.2155	-0.0322	N	0	0	0	0	0	0	0	0	0	0	0	0
3.1670	-0.5850	0.0449	C	0	0	0	0	0	0	0	0	0	0	0	0
3.8704	-0.2239	-0.7188	H	0	0	0	0	0	0	0	0	0	0	0	0
3.6236	-0.4625	1.0384	H	0	0	0	0	0	0	0	0	0	0	0	0
2.9490	-1.6422	-0.1297	H	0	0	0	0	0	0	0	0	0	0	0	0
0.7485	-0.3384	-0.1118	C	0	0	0	0	0	0	0	0	0	0	0	0
0.6728	-1.6440	0.0080	O	0	0	0	0	0	0	0	0	0	0	0	0
-0.2837	0.4140	-0.3183	O	0	0	0	0	0	0	0	0	0	0	0	0
-1.7318	0.1034	0.0304	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.4239	1.4077	-0.3435	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.4941	1.3327	-0.1023	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.9976	2.2488	0.2213	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.3212	1.6115	-1.4191	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.8072	-0.1797	1.5262	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.2525	-1.0862	1.8089	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.4214	0.6712	2.1057	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.8598	-0.3362	1.8043	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.2287	-1.0530	-0.8371	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.9337	-0.9212	-1.8879	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.9101	-2.0479	-0.4802	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.3275	-1.0758	-0.7968	H	0	0	0	0	0	0	0	0	0	0	0	0
-0.1902	-1.9903	-0.2794	H	0	0	0	0	0	0	0	0	0	0	0	0
2.1179	1.6706	-0.0347	C	0	0	0	0	0	0	0	0	0	0	0	0
2.5966	1.9817	-0.9756	H	0	0	0	0	0	0	0	0	0	0	0	0
1.1523	2.1731	0.0672	H	0	0	0	0	0	0	0	0	0	0	0	0
2.7705	1.9459	0.8058	H	0	0	0	0	0	0	0	0	0	0	0	0

1	2	1	0	0	0	0
1	6	2	0	0	0	0
1	23	1	0	0	0	0
2	3	1	0	0	0	0
2	4	1	0	0	0	0
2	5	1	0	0	0	0
6	7	4	0	0	0	0
6	8	4	0	0	0	0
7	22	1	0	0	0	0
9	10	1	0	0	0	0
9	14	1	0	0	0	0
9	18	1	0	0	0	0
10	11	1	0	0	0	0
10	12	1	0	0	0	0
10	13	1	0	0	0	0
14	15	1	0	0	0	0
14	16	1	0	0	0	0
14	17	1	0	0	0	0
18	19	1	0	0	0	0
18	20	1	0	0	0	0

18 21 1 0 0 0 0
23 24 1 0 0 0 0
23 25 1 0 0 0 0
23 26 1 0 0 0 0

Entry 3A Lewis acid = Mg++

Title Card Required

Created by GaussView 5.0.9
29 28 0 0 0 0 0 0 0 0 0 0
-0.6791 -0.8452 -0.1483 N 0 0 0 0 0 0 0 0 0 0 0 0
-0.4780 -2.3004 -0.3557 C 0 0 0 0 0 0 0 0 0 0 0 0
-1.4525 -2.7653 -0.5335 H 0 0 0 0 0 0 0 0 0 0 0 0
0.1554 -2.4554 -1.2371 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.0037 -2.7438 0.5289 H 0 0 0 0 0 0 0 0 0 0 0 0
0.4197 -0.0114 0.0112 C 0 0 0 0 0 0 0 0 0 0 0 0
0.3364 1.2235 0.1513 O 0 0 0 0 0 0 0 0 0 0 0 0
1.5247 -0.6793 -0.0063 O 0 0 0 0 0 0 0 0 0 0 0 0
-2.3064 -0.2945 -0.0658 S 0 0 0 0 0 0 0 0 0 0 0 0
-2.2938 1.1609 -0.4097 O 0 0 0 0 0 0 0 0 0 0 0 0
-3.1083 -1.1571 -0.9069 O 0 0 0 0 0 0 0 0 0 0 0 0
-2.7843 -0.4370 1.6437 C 0 0 0 0 0 0 0 0 0 0 0 0
-2.7225 -1.4949 1.9288 H 0 0 0 0 0 0 0 0 0 0 0 0
-2.1207 0.1893 2.2523 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.8234 -0.0821 1.6889 H 0 0 0 0 0 0 0 0 0 0 0 0
2.9266 -0.0960 0.0517 C 0 0 0 0 0 0 0 0 0 0 0 0
3.7857 -1.3496 -0.0673 C 0 0 0 0 0 0 0 0 0 0 0 0
4.8473 -1.0668 -0.0229 H 0 0 0 0 0 0 0 0 0 0 0 0
3.5769 -2.0468 0.7569 H 0 0 0 0 0 0 0 0 0 0 0 0
3.6025 -1.8637 -1.0222 H 0 0 0 0 0 0 0 0 0 0 0 0
3.1211 0.8347 -1.1408 C 0 0 0 0 0 0 0 0 0 0 0 0
2.8601 0.3267 -2.0811 H 0 0 0 0 0 0 0 0 0 0 0 0
2.5317 1.7561 -1.0489 H 0 0 0 0 0 0 0 0 0 0 0 0
4.1833 1.1163 -1.1944 H 0 0 0 0 0 0 0 0 0 0 0 0
3.1112 0.5909 1.3999 C 0 0 0 0 0 0 0 0 0 0 0 0
2.4762 1.4808 1.4984 H 0 0 0 0 0 0 0 0 0 0 0 0
2.8949 -0.1036 2.2251 H 0 0 0 0 0 0 0 0 0 0 0 0
4.1613 0.9064 1.4902 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.9829 2.6421 -0.2519 Mg 0 0 0 0 0 0 0 0 0 0 0 0
1 2 1 0 0 0 0
1 6 1 0 0 0 0
1 9 1 0 0 0 0
2 3 1 0 0 0 0
2 4 1 0 0 0 0
2 5 1 0 0 0 0

```
 6  7  2  0  0  0  0
 6  8  4  0  0  0  0
 7 29  1  0  0  0  0
 9 10  2  0  0  0  0
 9 11  2  0  0  0  0
 9 12  1  0  0  0  0
10 29  1  0  0  0  0
12 13  1  0  0  0  0
12 14  1  0  0  0  0
12 15  1  0  0  0  0
16 17  1  0  0  0  0
16 21  1  0  0  0  0
16 25  1  0  0  0  0
17 18  1  0  0  0  0
17 19  1  0  0  0  0
17 20  1  0  0  0  0
21 22  1  0  0  0  0
21 23  1  0  0  0  0
21 24  1  0  0  0  0
25 26  1  0  0  0  0
25 27  1  0  0  0  0
25 28  1  0  0  0  0
```

Entry 3B Lewis acid = Mg++

Title Card Required

```
Created by GaussView 5.0.9
 26 25  0  0  0  0  0  0  0  0  0  0    0
   1.5908    1.1074    0.0106 N   0  0  0  0  0  0  0  0  0  0  0  0
   1.3992    2.5379   -0.2357 C   0  0  0  0  0  0  0  0  0  0  0  0
   1.9695    2.8382   -1.1285 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.3401    2.7543   -0.3960 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.7627    3.1169    0.6270 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.5827    0.2287    0.0288 C   0  0  0  0  0  0  0  0  0  0  0  0
   0.7862   -1.0113    0.1916 O   0  0  0  0  0  0  0  0  0  0  0  0
  -0.6135    0.7410   -0.1261 O   0  0  0  0  0  0  0  0  0  0  0  0
  -1.9160    0.0254    0.0204 C   0  0  0  0  0  0  0  0  0  0  0  0
  -2.9238    1.1401   -0.2542 C   0  0  0  0  0  0  0  0  0  0  0  0
  -3.9461    0.7478   -0.1545 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.7957    1.9656    0.4609 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.8003    1.5341   -1.2738 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.0340   -1.0770   -1.0307 C   0  0  0  0  0  0  0  0  0  0  0  0
  -1.8057   -0.6844   -2.0328 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.3757   -1.9289   -0.8187 H   0  0  0  0  0  0  0  0  0  0  0  0
  -3.0696   -1.4481   -1.0418 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.0385   -0.4905    1.4527 C   0  0  0  0  0  0  0  0  0  0  0  0
```

-1.2930 -1.2660 1.6736 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.9204 0.3332 2.1726 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.0387 -0.9260 1.5954 H 0 0 0 0 0 0 0 0 0 0 0 0
1.6079 -2.6890 -0.1786 Mg 0 0 0 0 0 0 0 0 0 0 0 0
2.9619 0.6417 0.2010 C 0 0 0 0 0 0 0 0 0 0 0 0
3.0176 -0.0727 1.0333 H 0 0 0 0 0 0 0 0 0 0 0 0
3.3645 0.1722 -0.7122 H 0 0 0 0 0 0 0 0 0 0 0 0
3.5910 1.5052 0.4473 H 0 0 0 0 0 0 0 0 0 0 0 0
1 2 1 0 0 0 0
1 6 4 0 0 0 0
1 23 1 0 0 0 0
2 3 1 0 0 0 0
2 4 1 0 0 0 0
2 5 1 0 0 0 0
6 7 2 0 0 0 0
6 8 4 0 0 0 0
7 22 1 0 0 0 0
8 9 1 0 0 0 0
9 10 1 0 0 0 0
9 14 1 0 0 0 0
9 18 1 0 0 0 0
10 11 1 0 0 0 0
10 12 1 0 0 0 0
10 13 1 0 0 0 0
14 15 1 0 0 0 0
14 16 1 0 0 0 0
14 17 1 0 0 0 0
18 19 1 0 0 0 0
18 20 1 0 0 0 0
18 21 1 0 0 0 0
23 24 1 0 0 0 0
23 25 1 0 0 0 0
23 26 1 0 0 0 0

Entry 4A Lewis acid = $MoCl_3$

Title Card Required

Created by GaussView 5.0.9
32 30 0 0 0 0 0 0 0 0 0 0 0
1.4277 1.7213 0.2351 N 0 0 0 0 0 0 0 0 0 0 0 0
2.5433 2.4641 0.8526 C 0 0 0 0 0 0 0 0 0 0 0 0
2.1746 3.4465 1.1626 H 0 0 0 0 0 0 0 0 0 0 0 0
2.8909 1.9136 1.7351 H 0 0 0 0 0 0 0 0 0 0 0 0
3.3698 2.5808 0.1381 H 0 0 0 0 0 0 0 0 0 0 0 0
1.5604 0.3884 -0.1131 C 0 0 0 0 0 0 0 0 0 0 0 0

```
  0.6282   -0.2711   -0.5971 O   0  0  0  0  0  0  0  0  0  0  0  0
  2.7621   -0.0580    0.0949 O   0  0  0  0  0  0  0  0  0  0  0  0
 -0.0092    2.5771   -0.1926 S   0  0  0  0  0  0  0  0  0  0  0  0
 -1.1826    1.7288    0.1581 O   0  0  0  0  0  0  0  0  0  0  0  0
  0.0733    3.8819    0.4377 O   0  0  0  0  0  0  0  0  0  0  0  0
  0.0586    2.7256   -1.9687 C   0  0  0  0  0  0  0  0  0  0  0  0
  0.9455    3.3206   -2.2197 H   0  0  0  0  0  0  0  0  0  0  0  0
  0.0982    1.7202   -2.4057 H   0  0  0  0  0  0  0  0  0  0  0  0
 -0.8642    3.2468   -2.2588 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.1923   -1.4955   -0.0981 C   0  0  0  0  0  0  0  0  0  0  0  0
  4.6745   -1.4232    0.2538 C   0  0  0  0  0  0  0  0  0  0  0  0
  5.1197   -2.4249    0.1669 H   0  0  0  0  0  0  0  0  0  0  0  0
  5.2077   -0.7452   -0.4291 H   0  0  0  0  0  0  0  0  0  0  0  0
  4.8152   -1.0692    1.2857 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.4208   -2.3743    0.8817 C   0  0  0  0  0  0  0  0  0  0  0  0
  2.5286   -2.0002    1.9105 H   0  0  0  0  0  0  0  0  0  0  0  0
  1.3538   -2.4350    0.6331 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.8402   -3.3911    0.8423 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.9802   -1.8946   -1.5562 C   0  0  0  0  0  0  0  0  0  0  0  0
  1.9154   -1.9784   -1.8051 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.4589   -1.1709   -2.2333 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.4513   -2.8753   -1.7216 H   0  0  0  0  0  0  0  0  0  0  0  0
 -1.5242   -0.4720   -0.1429 Mo  0  0  0  0  0  0  0  0  0  0  0  0
 -1.5212   -2.7510   -0.8461 Cl  0  0  0  0  0  0  0  0  0  0  0  0
 -0.9338   -0.7874    2.1264 Cl  0  0  0  0  0  0  0  0  0  0  0  0
 -3.8959   -0.2376    0.0360 Cl  0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  6  1  0  0  0  0
 1  9  1  0  0  0  0
 2  3  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 6  7  2  0  0  0  0
 6  8  4  0  0  0  0
 8 16  1  0  0  0  0
 9 10  2  0  0  0  0
 9 11  2  0  0  0  0
 9 12  1  0  0  0  0
12 13  1  0  0  0  0
12 14  1  0  0  0  0
12 15  1  0  0  0  0
16 17  1  0  0  0  0
16 21  1  0  0  0  0
16 25  1  0  0  0  0
17 18  1  0  0  0  0
17 19  1  0  0  0  0
```

```
 17 20  1  0  0  0  0
 21 22  1  0  0  0  0
 21 23  1  0  0  0  0
 21 24  1  0  0  0  0
 25 26  1  0  0  0  0
 25 27  1  0  0  0  0
 25 28  1  0  0  0  0
 29 30  1  0  0  0  0
 29 31  1  0  0  0  0
 29 32  1  0  0  0  0
```

Entry 4B Lewis acid = $MoCl_3$

Title Card Required

Created by GaussView 5.0.9

```
 29 26  0  0  0  0  0  0  0  0  0    0
   -1.2068    2.1668   -0.5298 N   0  0  0  0  0  0  0  0  0  0  0  0
    0.0507    2.7803   -0.9515 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1765    3.5451   -1.7082 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.5631    3.2504   -0.0981 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.7182    2.0344   -1.3946 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3148    0.8527   -0.3079 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3405    0.0462   -0.3417 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5425    0.4303   -0.0900 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9672   -0.9864    0.0991 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.4847   -0.8389    0.2121 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.9461   -1.8289    0.3399 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.7538   -0.2148    1.0775 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.8975   -0.3761   -0.6965 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3786   -1.5457    1.3950 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3099   -1.7790    1.3047 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5318   -0.8416    2.2269 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9002   -2.4823    1.6446 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5871   -1.8101   -1.1317 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9542   -1.3248   -2.0491 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5029   -1.9609   -1.2082 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.0662   -2.7983   -1.0573 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.3345   -2.7291   -0.4294 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    2.8995    0.4326   -1.3725 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    1.5963    1.4114    1.9188 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -2.3472    3.0739   -0.4065 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7170    3.3679   -1.4027 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1583    2.6006    0.1533 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0212    3.9793    0.1264 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.5292   -0.4348    0.3444 Mo  0  0  0  0  0  0  0  0  0  0  0  0
```

```
 1  2  1  0  0  0  0
 1  6  4  0  0  0  0
 1 25  1  0  0  0  0
 2  3  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 6  7  2  0  0  0  0
 6  8  4  0  0  0  0
 7 29  1  0  0  0  0
 8  9  1  0  0  0  0
 9 10  1  0  0  0  0
 9 14  1  0  0  0  0
 9 18  1  0  0  0  0
10 11  1  0  0  0  0
10 12  1  0  0  0  0
10 13  1  0  0  0  0
14 15  1  0  0  0  0
14 16  1  0  0  0  0
14 17  1  0  0  0  0
18 19  1  0  0  0  0
18 20  1  0  0  0  0
18 21  1  0  0  0  0
23 29  1  0  0  0  0
25 26  1  0  0  0  0
25 27  1  0  0  0  0
25 28  1  0  0  0  0
```

Entry 5A Lewis acid = $FeCl_3$

Title Card Required

```
Created by GaussView 5.0.9
 29 27  0  0  0  0  0  0  0  0  0    0
   -1.1690    2.2250   -0.1793 N   0  0  0  0  0  0  0  0  0  0  0  0
    0.0721    2.9579   -0.4228 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1768    3.9284   -0.8734 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.6179    3.1272    0.5195 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.7204    2.4029   -1.1095 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2154    0.8930   -0.2990 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1949    0.2045   -0.5905 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4042    0.3580   -0.1373 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7204   -1.1007   -0.0988 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.2458   -1.0819   -0.0026 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.6278   -2.1119    0.0440 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.5732   -0.5477    0.9018 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.6844   -0.5862   -0.8814 H   0  0  0  0  0  0  0  0  0  0  0  0
```

-2.1012	-1.7170	1.1556	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.0077	-1.7888	1.0953	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.3765	-1.1363	2.0490	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.4930	-2.7380	1.2800	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.2619	-1.7837	-1.3874	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.6287	-1.2359	-2.2688	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.1702	-1.8688	-1.4428	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.6888	-2.7978	-1.4177	H	0	0	0	0	0	0	0	0	0	0	0	0
1.5931	-0.3079	0.0289	Fe	0	0	0	0	0	0	0	0	0	0	0	0
1.6995	-2.5209	-0.1472	Cl	0	0	0	0	0	0	0	0	0	0	0	0
3.0828	0.7248	-1.2566	Cl	0	0	0	0	0	0	0	0	0	0	0	0
1.6436	0.4082	2.1329	Cl	0	0	0	0	0	0	0	0	0	0	0	0
-2.3216	3.0257	0.2277	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.6638	3.6528	-0.6115	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.1410	2.3792	0.5524	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.0277	3.6844	1.0593	H	0	0	0	0	0	0	0	0	0	0	0	0

1	2	1	0	0	0	0
1	6	4	0	0	0	0
1	26	1	0	0	0	0
2	3	1	0	0	0	0
2	4	1	0	0	0	0
2	5	1	0	0	0	0
6	7	2	0	0	0	0
6	8	4	0	0	0	0
8	9	1	0	0	0	0
9	10	1	0	0	0	0
9	14	1	0	0	0	0
9	18	1	0	0	0	0
10	11	1	0	0	0	0
10	12	1	0	0	0	0
10	13	1	0	0	0	0
14	15	1	0	0	0	0
14	16	1	0	0	0	0
14	17	1	0	0	0	0
18	19	1	0	0	0	0
18	20	1	0	0	0	0
18	21	1	0	0	0	0
22	23	1	0	0	0	0
22	24	1	0	0	0	0
22	25	1	0	0	0	0
26	27	1	0	0	0	0
26	28	1	0	0	0	0
26	29	1	0	0	0	0

Entry 5B Lewis acid = $FeCl_3$

Title Card Required

Created by GaussView 5.0.9
```
 29 27  0  0  0  0  0  0  0  0  0    0
   -1.1690    2.2250   -0.1793 N   0  0  0  0  0  0  0  0  0  0  0  0
    0.0721    2.9579   -0.4228 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1768    3.9284   -0.8734 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.6179    3.1272    0.5195 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.7204    2.4029   -1.1095 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2154    0.8930   -0.2990 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1949    0.2045   -0.5905 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4042    0.3580   -0.1373 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7204   -1.1007   -0.0988 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.2458   -1.0819   -0.0026 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.6278   -2.1119    0.0440 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.5732   -0.5477    0.9018 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.6844   -0.5862   -0.8814 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1012   -1.7170    1.1556 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0077   -1.7888    1.0953 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3765   -1.1363    2.0490 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4930   -2.7380    1.2800 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2619   -1.7837   -1.3874 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6287   -1.2359   -2.2688 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1702   -1.8688   -1.4428 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6888   -2.7978   -1.4177 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.5931   -0.3079    0.0289 Fe  0  0  0  0  0  0  0  0  0  0  0  0
    1.6995   -2.5209   -0.1472 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    3.0828    0.7248   -1.2566 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    1.6436    0.4082    2.1329 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -2.3216    3.0257    0.2277 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6638    3.6528   -0.6115 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1410    2.3792    0.5524 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0277    3.6844    1.0593 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  6  4  0  0  0  0
  1 26  1  0  0  0  0
  2  3  1  0  0  0  0
  2  4  1  0  0  0  0
  2  5  1  0  0  0  0
  6  7  2  0  0  0  0
  6  8  4  0  0  0  0
  8  9  1  0  0  0  0
  9 10  1  0  0  0  0
  9 14  1  0  0  0  0
  9 18  1  0  0  0  0
 10 11  1  0  0  0  0
```

10 12 1 0 0 0 0
10 13 1 0 0 0 0
14 15 1 0 0 0 0
14 16 1 0 0 0 0
14 17 1 0 0 0 0
18 19 1 0 0 0 0
18 20 1 0 0 0 0
18 21 1 0 0 0 0
22 23 1 0 0 0 0
22 24 1 0 0 0 0
22 25 1 0 0 0 0
26 27 1 0 0 0 0
26 28 1 0 0 0 0
26 29 1 0 0 0 0

Entry 6A Lewis acid = $AuCl_3$

Title Card Required

Created by GaussView 5.0.9
32 30 0 0 0 0 0 0 0 0 0 0
-2.0597 1.3064 -0.4113 N 0 0 0 0 0 0 0 0 0 0 0 0
-3.3274 1.5638 -1.1126 C 0 0 0 0 0 0 0 0 0 0 0 0
-3.3136 2.5950 -1.4772 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.4169 0.8749 -1.9623 H 0 0 0 0 0 0 0 0 0 0 0 0
-4.1799 1.4216 -0.4336 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.7539 0.0556 0.0329 C 0 0 0 0 0 0 0 0 0 0 0 0
-0.6834 -0.2217 0.6304 O 0 0 0 0 0 0 0 0 0 0 0 0
-2.7218 -0.7973 -0.1432 O 0 0 0 0 0 0 0 0 0 0 0 0
-0.9921 2.6752 -0.0631 S 0 0 0 0 0 0 0 0 0 0 0 0
0.3345 2.3727 -0.5947 O 0 0 0 0 0 0 0 0 0 0 0 0
-1.7274 3.8348 -0.5571 O 0 0 0 0 0 0 0 0 0 0 0 0
-0.9320 2.7240 1.7225 C 0 0 0 0 0 0 0 0 0 0 0 0
-1.9572 2.8231 2.0995 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.4250 1.8237 2.0905 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.3414 3.6219 1.9525 H 0 0 0 0 0 0 0 0 0 0 0 0
-2.7445 -2.2222 0.3504 C 0 0 0 0 0 0 0 0 0 0 0 0
-4.1053 -2.6995 -0.1491 C 0 0 0 0 0 0 0 0 0 0 0 0
-4.2732 -3.7349 0.1809 H 0 0 0 0 0 0 0 0 0 0 0 0
-4.9125 -2.0704 0.2538 H 0 0 0 0 0 0 0 0 0 0 0 0
-4.1502 -2.6727 -1.2479 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.6098 -3.0165 -0.2889 C 0 0 0 0 0 0 0 0 0 0 0 0
-1.5775 -2.8508 -1.3750 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.6319 -2.7586 0.1346 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.7882 -4.0870 -0.1069 H 0 0 0 0 0 0 0 0 0 0 0 0
-2.6798 -2.2052 1.8758 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.7162 -1.8220 2.2361 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.4929 -1.5938 2.2954 H 0 0 0 0 0 0 0 0 0 0 0 0
-2.8016 -3.2342 2.2464 H 0 0 0 0 0 0 0 0 0 0 0 0
1.3457 -0.3272 -0.0196 Au 0 0 0 0 0 0 0 0 0 0 0 0
1.9513 0.0711 2.2132 Cl 0 0 0 0 0 0 0 0 0 0 0 0
3.5397 -0.5675 -0.6254 Cl 0 0 0 0 0 0 0 0 0 0 0 0
0.6420 -0.7474 -2.2182 Cl 0 0 0 0 0 0 0 0 0 0 0 0
1 2 1 0 0 0 0
1 6 4 0 0 0 0
1 9 1 0 0 0 0
2 3 1 0 0 0 0
2 4 1 0 0 0 0
2 5 1 0 0 0 0
6 7 2 0 0 0 0
6 8 4 0 0 0 0
8 16 1 0 0 0 0
9 10 2 0 0 0 0
9 11 2 0 0 0 0
9 12 1 0 0 0 0
12 13 1 0 0 0 0
12 14 1 0 0 0 0
12 15 1 0 0 0 0
16 17 1 0 0 0 0
16 21 1 0 0 0 0
16 25 1 0 0 0 0
17 18 1 0 0 0 0
17 19 1 0 0 0 0
17 20 1 0 0 0 0
21 22 1 0 0 0 0
21 23 1 0 0 0 0
21 24 1 0 0 0 0
25 26 1 0 0 0 0
25 27 1 0 0 0 0
25 28 1 0 0 0 0
29 30 1 0 0 0 0
29 31 1 0 0 0 0
29 32 1 0 0 0 0

Entry 6B Lewis acid = $AuCl_3$

Title Card Required

Created by GaussView 5.0.9
29 28 0 0 0 0 0 0 0 0 0 0 0
-1.6700 1.8699 -0.8929 N 0 0 0 0 0 0 0 0 0 0 0 0
-0.5007 2.4229 -1.5696 C 0 0 0 0 0 0 0 0 0 0 0 0

```
 -0.8348    3.2188   -2.2493 H   0  0  0  0  0  0  0  0  0  0  0  0
  0.2100    2.8484   -0.8423 H   0  0  0  0  0  0  0  0  0  0  0  0
  0.0014    1.6482   -2.1600 H   0  0  0  0  0  0  0  0  0  0  0  0
 -1.7237    0.5772   -0.5586 C   0  0  0  0  0  0  0  0  0  0  0  0
 -0.7582   -0.2329   -0.7352 O   0  0  0  0  0  0  0  0  0  0  0  0
 -2.8832    0.1666   -0.0982 O   0  0  0  0  0  0  0  0  0  0  0  0
 -3.1881   -1.2146    0.3801 C   0  0  0  0  0  0  0  0  0  0  0  0
 -4.6147   -1.0580    0.9045 C   0  0  0  0  0  0  0  0  0  0  0  0
 -4.9904   -2.0317    1.2510 H   0  0  0  0  0  0  0  0  0  0  0  0
 -4.6456   -0.3530    1.7488 H   0  0  0  0  0  0  0  0  0  0  0  0
 -5.2822   -0.6880    0.1124 H   0  0  0  0  0  0  0  0  0  0  0  0
 -2.2351   -1.6157    1.5057 C   0  0  0  0  0  0  0  0  0  0  0  0
 -1.2307   -1.8496    1.1332 H   0  0  0  0  0  0  0  0  0  0  0  0
 -2.1570   -0.8149    2.2555 H   0  0  0  0  0  0  0  0  0  0  0  0
 -2.6337   -2.5138    2.0011 H   0  0  0  0  0  0  0  0  0  0  0  0
 -3.1363   -2.1698   -0.8115 C   0  0  0  0  0  0  0  0  0  0  0  0
 -3.8165   -1.8334   -1.6088 H   0  0  0  0  0  0  0  0  0  0  0  0
 -2.1194   -2.2490   -1.2174 H   0  0  0  0  0  0  0  0  0  0  0  0
 -3.4594   -3.1702   -0.4859 H   0  0  0  0  0  0  0  0  0  0  0  0
 -2.7340    2.8139   -0.5566 C   0  0  0  0  0  0  0  0  0  0  0  0
 -3.2706    3.1286   -1.4661 H   0  0  0  0  0  0  0  0  0  0  0  0
 -3.4428    2.3562    0.1389 H   0  0  0  0  0  0  0  0  0  0  0  0
 -2.2870    3.7023   -0.0856 H   0  0  0  0  0  0  0  0  0  0  0  0
  1.1896   -0.1016    0.0353 Au  0  0  0  0  0  0  0  0  0  0  0  0
  0.4172    1.2583    1.7897 Cl  0  0  0  0  0  0  0  0  0  0  0  0
  3.3210   -0.0758    0.8939 Cl  0  0  0  0  0  0  0  0  0  0  0  0
  1.8854   -1.4454   -1.7518 Cl  0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  6  4  0  0  0  0
 1 22  1  0  0  0  0
 2  3  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 6  7  2  0  0  0  0
 6  8  4  0  0  0  0
 7 26  1  0  0  0  0
 8  9  1  0  0  0  0
 9 10  1  0  0  0  0
 9 14  1  0  0  0  0
 9 18  1  0  0  0  0
10 11  1  0  0  0  0
10 12  1  0  0  0  0
10 13  1  0  0  0  0
14 15  1  0  0  0  0
14 16  1  0  0  0  0
14 17  1  0  0  0  0
```

18 19 1 0 0 0 0
18 20 1 0 0 0 0
18 21 1 0 0 0 0
22 23 1 0 0 0 0
22 24 1 0 0 0 0
22 25 1 0 0 0 0
26 27 1 0 0 0 0
26 28 1 0 0 0 0
26 29 1 0 0 0 0

Entry 7A Lewis acid = $InCl_3$

Title Card Required

Created by GaussView 5.0.9
32 31 0 0 0 0 0 0 0 0 0 0
1.5979 1.7743 0.2101 N 0 0 0 0 0 0 0 0 0 0 0 0
2.8070 2.5249 0.5931 C 0 0 0 0 0 0 0 0 0 0 0 0
2.5193 3.5625 0.7878 H 0 0 0 0 0 0 0 0 0 0 0 0
3.2365 2.0917 1.5056 H 0 0 0 0 0 0 0 0 0 0 0 0
3.5477 2.4877 -0.2169 H 0 0 0 0 0 0 0 0 0 0 0 0
1.6468 0.4216 -0.0435 C 0 0 0 0 0 0 0 0 0 0 0 0
0.6542 -0.2456 -0.3791 O 0 0 0 0 0 0 0 0 0 0 0 0
2.8522 -0.0552 0.0754 O 0 0 0 0 0 0 0 0 0 0 0 0
0.0872 2.6133 0.0673 S 0 0 0 0 0 0 0 0 0 0 0 0
-0.9516 1.7311 0.6374 O 0 0 0 0 0 0 0 0 0 0 0 0
0.2895 3.9232 0.6667 O 0 0 0 0 0 0 0 0 0 0 0 0
-0.1640 2.7736 -1.6912 C 0 0 0 0 0 0 0 0 0 0 0 0
0.6666 3.3658 -2.0944 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.2238 1.7736 -2.1363 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.1218 3.2992 -1.8057 H 0 0 0 0 0 0 0 0 0 0 0 0
3.2327 -1.5039 -0.1047 C 0 0 0 0 0 0 0 0 0 0 0 0
4.7403 -1.4571 0.1245 C 0 0 0 0 0 0 0 0 0 0 0 0
5.1575 -2.4695 0.0238 H 0 0 0 0 0 0 0 0 0 0 0 0
5.2288 -0.8045 -0.6142 H 0 0 0 0 0 0 0 0 0 0 0 0
4.9715 -1.0842 1.1332 H 0 0 0 0 0 0 0 0 0 0 0 0
2.5273 -2.3376 0.9616 C 0 0 0 0 0 0 0 0 0 0 0 0
2.7047 -1.9198 1.9642 H 0 0 0 0 0 0 0 0 0 0 0 0
1.4480 -2.4116 0.7777 H 0 0 0 0 0 0 0 0 0 0 0 0
2.9423 -3.3567 0.9410 H 0 0 0 0 0 0 0 0 0 0 0 0
2.8940 -1.9427 -1.5271 C 0 0 0 0 0 0 0 0 0 0 0 0
1.8107 -2.0075 -1.6873 H 0 0 0 0 0 0 0 0 0 0 0 0
3.3346 -1.2536 -2.2635 H 0 0 0 0 0 0 0 0 0 0 0 0
3.3264 -2.9405 -1.6964 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.1737 -2.9359 -0.5580 Cl 0 0 0 0 0 0 0 0 0 0 0 0
-2.2522 -0.6756 2.3420 Cl 0 0 0 0 0 0 0 0 0 0 0 0

-2.8278 0.3428 -1.6916 Cl 0 0 0 0 0 0 0 0 0 0 0 0
-1.5240 -0.6265 0.0691 In 0 0 0 0 0 0 0 0 0 0 0 0
1 2 1 0 0 0 0
1 6 4 0 0 0 0
1 9 1 0 0 0 0
2 3 1 0 0 0 0
2 4 1 0 0 0 0
2 5 1 0 0 0 0
6 7 2 0 0 0 0
6 8 4 0 0 0 0
7 32 1 0 0 0 0
8 16 1 0 0 0 0
9 10 2 0 0 0 0
9 11 2 0 0 0 0
9 12 1 0 0 0 0
12 13 1 0 0 0 0
12 14 1 0 0 0 0
12 15 1 0 0 0 0
16 17 1 0 0 0 0
16 21 1 0 0 0 0
16 25 1 0 0 0 0
17 18 1 0 0 0 0
17 19 1 0 0 0 0
17 20 1 0 0 0 0
21 22 1 0 0 0 0
21 23 1 0 0 0 0
21 24 1 0 0 0 0
25 26 1 0 0 0 0
25 27 1 0 0 0 0
25 28 1 0 0 0 0
29 32 1 0 0 0 0
30 32 1 0 0 0 0
31 32 1 0 0 0 0

Entry 7B Lewis acid = $InCl_3$

Title Card Required

Created by GaussView 5.0.9
29 28 0 0 0 0 0 0 0 0 0 0
-1.4859 2.2056 -0.1411 N 0 0 0 0 0 0 0 0 0 0 0 0
-0.2425 2.9222 -0.4138 C 0 0 0 0 0 0 0 0 0 0 0 0
-0.4918 3.9020 -0.8436 H 0 0 0 0 0 0 0 0 0 0 0 0
0.3399 3.0773 0.5090 H 0 0 0 0 0 0 0 0 0 0 0 0
0.3692 2.3754 -1.1413 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.5441 0.8701 -0.2392 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.5393	0.1528	-0.5005	O	0	0	0	0	0	0	0	0	0	0	0
-2.7474	0.3586	-0.0839	O	0	0	0	0	0	0	0	0	0	0	0
-3.0803	-1.0939	-0.0821	C	0	0	0	0	0	0	0	0	0	0	0
-4.5923	-1.0689	0.1396	C	0	0	0	0	0	0	0	0	0	0	0
-4.9839	-2.0964	0.1485	H	0	0	0	0	0	0	0	0	0	0	0
-4.8375	-0.5951	1.1019	H	0	0	0	0	0	0	0	0	0	0	0
-5.0945	-0.5110	-0.6647	H	0	0	0	0	0	0	0	0	0	0	0
-2.3699	-1.7876	1.0799	C	0	0	0	0	0	0	0	0	0	0	0
-1.2926	-1.8962	0.9032	H	0	0	0	0	0	0	0	0	0	0	0
-2.5330	-1.2365	2.0186	H	0	0	0	0	0	0	0	0	0	0	0
-2.7907	-2.7972	1.2026	H	0	0	0	0	0	0	0	0	0	0	0
-2.7327	-1.7055	-1.4393	C	0	0	0	0	0	0	0	0	0	0	0
-3.1993	-1.1310	-2.2541	H	0	0	0	0	0	0	0	0	0	0	0
-1.6484	-1.7434	-1.6006	H	0	0	0	0	0	0	0	0	0	0	0
-3.1251	-2.7330	-1.4791	H	0	0	0	0	0	0	0	0	0	0	0
1.5142	-2.6280	0.1385	Cl	0	0	0	0	0	0	0	0	0	0	0
2.7545	0.6706	-1.7721	Cl	0	0	0	0	0	0	0	0	0	0	0
1.8170	0.8597	2.1374	Cl	0	0	0	0	0	0	0	0	0	0	0
1.5194	-0.2482	0.0482	In	0	0	0	0	0	0	0	0	0	0	0
-2.6320	3.0234	0.2509	C	0	0	0	0	0	0	0	0	0	0	0
-2.9881	3.6199	-0.6049	H	0	0	0	0	0	0	0	0	0	0	0
-3.4469	2.3904	0.6118	H	0	0	0	0	0	0	0	0	0	0	0
-2.3266	3.7116	1.0540	H	0	0	0	0	0	0	0	0	0	0	0

1	2	1	0	0	0	0
1	6	4	0	0	0	0
1	26	1	0	0	0	0
2	3	1	0	0	0	0
2	4	1	0	0	0	0
2	5	1	0	0	0	0
6	7	2	0	0	0	0
6	8	4	0	0	0	0
7	25	1	0	0	0	0
8	9	1	0	0	0	0
9	10	1	0	0	0	0
9	14	1	0	0	0	0
9	18	1	0	0	0	0
10	11	1	0	0	0	0
10	12	1	0	0	0	0
10	13	1	0	0	0	0
14	15	1	0	0	0	0
14	16	1	0	0	0	0
14	17	1	0	0	0	0
18	19	1	0	0	0	0
18	20	1	0	0	0	0
18	21	1	0	0	0	0
22	25	1	0	0	0	0

23 25 1 0 0 0 0
24 25 1 0 0 0 0
26 27 1 0 0 0 0
26 28 1 0 0 0 0
26 29 1 0 0 0 0

Entry 8A Lewis acid = $MgCl_2$

Title Card Required

Created by GaussView 5.0.9

31 31 0 0 0 0 0 0 0 0 0 0

-0.2169	1.7072	-0.2696	N	0	0	0	0	0	0	0	0	0	0	0	0	
-0.9664	2.9482	-0.5479	C	0	0	0	0	0	0	0	0	0	0	0	0	
-0.2518	3.7414	-0.7873	H	0	0	0	0	0	0	0	0	0	0	0	0	
-1.6326	2.7955	-1.4069	H	0	0	0	0	0	0	0	0	0	0	0	0	
-1.5579	3.2325	0.3318	H	0	0	0	0	0	0	0	0	0	0	0	0	
-0.8849	0.5383	0.0697	C	0	0	0	0	0	0	0	0	0	0	0	0	
-0.3112	-0.5220	0.3278	O	0	0	0	0	0	0	0	0	0	0	0	0	
-2.1770	0.7190	0.0877	O	0	0	0	0	0	0	0	0	0	0	0	0	
1.5033	1.7488	-0.3932	S	0	0	0	0	0	0	0	0	0	0	0	0	
1.9457	0.4119	-0.8666	O	0	0	0	0	0	0	0	0	0	0	0	0	
1.8318	2.8973	-1.2211	O	0	0	0	0	0	0	0	0	0	0	0	0	
2.0986	1.9928	1.2692	C	0	0	0	0	0	0	0	0	0	0	0	0	
1.5851	2.8683	1.6854	H	0	0	0	0	0	0	0	0	0	0	0	0	
1.9328	1.0716	1.8461	H	0	0	0	0	0	0	0	0	0	0	0	0	
3.1758	2.1833	1.1613	H	0	0	0	0	0	0	0	0	0	0	0	0	
2.5591	-1.5516	1.9104	Cl	0	0	0	0	0	0	0	0	0	0	0	0	
0.9561	-3.0373	-1.7431	Cl	0	0	0	0	0	0	0	0	0	0	0	0	
-3.1814	-0.3760	0.3264	C	0	0	0	0	0	0	0	0	0	0	0	0	
-4.5017	0.3850	0.2431	C	0	0	0	0	0	0	0	0	0	0	0	0	
-5.3382	-0.3130	0.3922	H	0	0	0	0	0	0	0	0	0	0	0	0	
-4.5551	1.1628	1.0192	H	0	0	0	0	0	0	0	0	0	0	0	0	
-4.6173	0.8607	-0.7420	H	0	0	0	0	0	0	0	0	0	0	0	0	
-3.0601	-1.4069	-0.7937	C	0	0	0	0	0	0	0	0	0	0	0	0	
-3.1674	-0.9246	-1.7771	H	0	0	0	0	0	0	0	0	0	0	0	0	
-2.1037	-1.9452	-0.7630	H	0	0	0	0	0	0	0	0	0	0	0	0	
-3.8711	-2.1430	-0.6866	H	0	0	0	0	0	0	0	0	0	0	0	0	
-2.9673	-0.9682	1.7175	C	0	0	0	0	0	0	0	0	0	0	0	0	
-2.0270	-1.5291	1.7836	H	0	0	0	0	0	0	0	0	0	0	0	0	
-2.9699	-0.1761	2.4817	H	0	0	0	0	0	0	0	0	0	0	0	0	
-3.7971	-1.6561	1.9391	H	0	0	0	0	0	0	0	0	0	0	0	0	
1.4472	-1.4899	-0.1225	Mg	0	0	0	0	0	0	0	0	0	0	0	0	

1 2 1 0 0 0 0
1 6 1 0 0 0 0
1 9 1 0 0 0 0
2 3 1 0 0 0 0

```
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 6  7  2  0  0  0  0
 6  8  4  0  0  0  0
 7 31  1  0  0  0  0
 8 18  1  0  0  0  0
 9 10  2  0  0  0  0
 9 11  2  0  0  0  0
 9 12  1  0  0  0  0
10 31  1  0  0  0  0
12 13  1  0  0  0  0
12 14  1  0  0  0  0
12 15  1  0  0  0  0
16 31  1  0  0  0  0
17 31  1  0  0  0  0
18 19  1  0  0  0  0
18 23  1  0  0  0  0
18 27  1  0  0  0  0
19 20  1  0  0  0  0
19 21  1  0  0  0  0
19 22  1  0  0  0  0
23 24  1  0  0  0  0
23 25  1  0  0  0  0
23 26  1  0  0  0  0
27 28  1  0  0  0  0
27 29  1  0  0  0  0
27 30  1  0  0  0  0
```

Entry 8B Lewis acid = $MgCl_2$

Title Card Required

Created by GaussView 5.0.9

```
28 27  0  0  0  0  0  0  0  0  0  0    0
  -0.9073    2.0792   -0.5697 N   0  0  0  0  0  0  0  0  0  0  0  0
  -2.1305    2.8299   -0.8365 C   0  0  0  0  0  0  0  0  0  0  0  0
  -2.1402    3.1760   -1.8825 H   0  0  0  0  0  0  0  0  0  0  0  0
  -3.0048    2.1968   -0.6630 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.1883    3.7104   -0.1766 H   0  0  0  0  0  0  0  0  0  0  0  0
  -0.8943    0.8006   -0.1570 C   0  0  0  0  0  0  0  0  0  0  0  0
   0.1739    0.1788    0.0294 O   0  0  0  0  0  0  0  0  0  0  0  0
  -2.0882    0.2680    0.0367 O   0  0  0  0  0  0  0  0  0  0  0  0
   3.3626    0.7461    1.5811 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   2.4559   -1.9471   -1.5615 Cl  0  0  0  0  0  0  0  0  0  0  0  0
  -2.3355   -1.1355    0.4538 C   0  0  0  0  0  0  0  0  0  0  0  0
  -3.8623   -1.1862    0.5184 C   0  0  0  0  0  0  0  0  0  0  0  0
```

-4.1901	-2.1910	0.8227	H	0	0	0	0	0	0	0	0	0	0	0
-4.2455	-0.4585	1.2494	H	0	0	0	0	0	0	0	0	0	0	0
-4.3012	-0.9598	-0.4648	H	0	0	0	0	0	0	0	0	0	0	0
-1.8054	-2.0944	-0.6131	C	0	0	0	0	0	0	0	0	0	0	0
-2.2206	-1.8390	-1.6001	H	0	0	0	0	0	0	0	0	0	0	0
-0.7098	-2.0838	-0.6770	H	0	0	0	0	0	0	0	0	0	0	0
-2.1248	-3.1183	-0.3661	H	0	0	0	0	0	0	0	0	0	0	0
-1.7278	-1.3841	1.8350	C	0	0	0	0	0	0	0	0	0	0	0
-0.6311	-1.3756	1.8093	H	0	0	0	0	0	0	0	0	0	0	0
-2.0732	-0.6233	2.5516	H	0	0	0	0	0	0	0	0	0	0	0
-2.0557	-2.3692	2.2001	H	0	0	0	0	0	0	0	0	0	0	0
2.0706	-0.3410	0.0319	Mg	0	0	0	0	0	0	0	0	0	0	0
0.3708	2.7526	-0.7871	C	0	0	0	0	0	0	0	0	0	0	0
0.9923	2.7307	0.1202	H	0	0	0	0	0	0	0	0	0	0	0
0.9341	2.2889	-1.6132	H	0	0	0	0	0	0	0	0	0	0	0
0.1727	3.7989	-1.0482	H	0	0	0	0	0	0	0	0	0	0	0

1	2	1	0	0	0	0
1	6	4	0	0	0	0
1	25	1	0	0	0	0
2	3	1	0	0	0	0
2	4	1	0	0	0	0
2	5	1	0	0	0	0
6	7	2	0	0	0	0
6	8	4	0	0	0	0
7	24	1	0	0	0	0
8	11	1	0	0	0	0
9	24	1	0	0	0	0
10	24	1	0	0	0	0
11	12	1	0	0	0	0
11	16	1	0	0	0	0
11	20	1	0	0	0	0
12	13	1	0	0	0	0
12	14	1	0	0	0	0
12	15	1	0	0	0	0
16	17	1	0	0	0	0
16	18	1	0	0	0	0
16	19	1	0	0	0	0
20	21	1	0	0	0	0
20	22	1	0	0	0	0
20	23	1	0	0	0	0
25	26	1	0	0	0	0
25	27	1	0	0	0	0
25	28	1	0	0	0	0

Entry 9A Lewis acid = $RuCl_3$

Title Card Required

Created by GaussView 5.0.9
32 27 0 0 0 0 0 0 0 0 0 0
1.5694 -1.0841 -0.5044 N 0 0 0 0 0 0 0 0 0 0 0 0
0.7239 -2.2115 -0.9212 C 0 0 0 0 0 0 0 0 0 0 0 0
1.3661 -3.0144 -1.2972 H 0 0 0 0 0 0 0 0 0 0 0 0
0.1237 -2.5956 -0.0839 H 0 0 0 0 0 0 0 0 0 0 0 0
0.0603 -1.8728 -1.7264 H 0 0 0 0 0 0 0 0 0 0 0 0
1.0818 0.1962 -0.5080 C 0 0 0 0 0 0 0 0 0 0 0 0
-0.1223 0.4562 -0.6881 O 0 0 0 0 0 0 0 0 0 0 0 0
2.0149 1.1014 -0.3666 O 0 0 0 0 0 0 0 0 0 0 0 0
1.7825 2.5532 -0.0658 C 0 0 0 0 0 0 0 0 0 0 0 0
3.2067 3.0574 0.1560 C 0 0 0 0 0 0 0 0 0 0 0 0
3.1851 4.1260 0.4141 H 0 0 0 0 0 0 0 0 0 0 0 0
3.6867 2.5061 0.9776 H 0 0 0 0 0 0 0 0 0 0 0 0
3.8123 2.9342 -0.7544 H 0 0 0 0 0 0 0 0 0 0 0 0
0.9479 2.6784 1.2070 C 0 0 0 0 0 0 0 0 0 0 0 0
-0.0956 2.3720 1.0560 H 0 0 0 0 0 0 0 0 0 0 0 0
1.3903 2.0811 2.0183 H 0 0 0 0 0 0 0 0 0 0 0 0
0.9440 3.7324 1.5230 H 0 0 0 0 0 0 0 0 0 0 0 0
1.1331 3.2144 -1.2788 C 0 0 0 0 0 0 0 0 0 0 0 0
1.7294 3.0328 -2.1858 H 0 0 0 0 0 0 0 0 0 0 0 0
0.1110 2.8488 -1.4407 H 0 0 0 0 0 0 0 0 0 0 0 0
1.0905 4.3014 -1.1114 H 0 0 0 0 0 0 0 0 0 0 0 0
3.1045 -1.4680 0.2734 S 0 0 0 0 0 0 0 0 0 0 0 0
3.2092 -0.6737 1.4935 O 0 0 0 0 0 0 0 0 0 0 0 0
3.1077 -2.9276 0.3446 O 0 0 0 0 0 0 0 0 0 0 0 0
4.3320 -0.9395 -0.9133 C 0 0 0 0 0 0 0 0 0 0 0 0
4.1795 -1.5067 -1.8397 H 0 0 0 0 0 0 0 0 0 0 0 0
4.2310 0.1401 -1.0673 H 0 0 0 0 0 0 0 0 0 0 0 0
5.3007 -1.1878 -0.4579 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.0775 1.9123 0.6736 Cl 0 0 0 0 0 0 0 0 0 0 0 0
-3.1732 -1.0436 -1.9128 Cl 0 0 0 0 0 0 0 0 0 0 0 0
-2.1116 -1.6865 1.8740 Cl 0 0 0 0 0 0 0 0 0 0 0 0
-2.1486 -0.1787 0.0459 Ru 0 0 0 0 0 0 0 0 0 0 0 0
1 2 1 0 0 0 0
1 6 4 0 0 0 0
1 22 1 0 0 0 0
2 3 1 0 0 0 0
2 4 1 0 0 0 0
2 5 1 0 0 0 0
6 7 2 0 0 0 0
6 8 4 0 0 0 0
8 9 1 0 0 0 0
9 10 1 0 0 0 0

```
 9 14  1  0  0  0  0
 9 18  1  0  0  0  0
10 11  1  0  0  0  0
10 12  1  0  0  0  0
10 13  1  0  0  0  0
14 15  1  0  0  0  0
14 16  1  0  0  0  0
14 17  1  0  0  0  0
18 19  1  0  0  0  0
18 20  1  0  0  0  0
18 21  1  0  0  0  0
22 23  2  0  0  0  0
22 24  2  0  0  0  0
22 25  1  0  0  0  0
25 26  1  0  0  0  0
25 27  1  0  0  0  0
25 28  1  0  0  0  0
```

Entry 9B Lewis acid = $RuCl_3$

Title Card Required

Created by GaussView 5.0.9

```
 29 24  0  0  0  0  0  0  0  0  0    0
   -1.4760    2.2450   -0.1776 N   0  0  0  0  0  0  0  0  0  0  0  0
   -0.2208    2.9507   -0.4266 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.4568    3.9557   -0.8011 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.3754    3.0477    0.4958 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.3769    2.4300   -1.1839 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5242    0.9053   -0.2360 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5092    0.1939   -0.4547 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7285    0.3889   -0.0827 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.0390   -1.0649   -0.0084 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.5598   -1.0538    0.1449 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.9348   -2.0853    0.2117 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.8565   -0.5159    1.0579 H   0  0  0  0  0  0  0  0  0  0  0  0
   -5.0340   -0.5655   -0.7196 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3682   -1.6690    1.2254 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2797   -1.7446    1.1073 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5986   -1.0737    2.1222 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7588   -2.6857    1.3833 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6243   -1.7600   -1.3058 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.0369   -1.2301   -2.1780 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5337   -1.8234   -1.4033 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.0310   -2.7829   -1.3065 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.3808   -2.6492   -0.1657 Cl  0  0  0  0  0  0  0  0  0  0  0  0
```

2.8493 0.7368 -1.6532 Cl 0 0 0 0 0 0 0 0 0 0 0 0
2.0931 0.6744 2.1679 Cl 0 0 0 0 0 0 0 0 0 0 0 0
1.5479 -0.2814 0.0621 Ru 0 0 0 0 0 0 0 0 0 0 0 0
-2.6336 3.0688 0.1627 C 0 0 0 0 0 0 0 0 0 0 0 0
-2.9483 3.6655 -0.7090 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.4669 2.4396 0.4862 H 0 0 0 0 0 0 0 0 0 0 0 0
-2.3637 3.7577 0.9781 H 0 0 0 0 0 0 0 0 0 0 0 0
1 2 1 0 0 0 0
1 6 4 0 0 0 0
1 26 1 0 0 0 0
2 3 1 0 0 0 0
2 4 1 0 0 0 0
2 5 1 0 0 0 0
6 7 2 0 0 0 0
6 8 4 0 0 0 0
8 9 1 0 0 0 0
9 10 1 0 0 0 0
9 14 1 0 0 0 0
9 18 1 0 0 0 0
10 11 1 0 0 0 0
10 12 1 0 0 0 0
10 13 1 0 0 0 0
14 15 1 0 0 0 0
14 16 1 0 0 0 0
14 17 1 0 0 0 0
18 19 1 0 0 0 0
18 20 1 0 0 0 0
18 21 1 0 0 0 0
26 27 1 0 0 0 0
26 28 1 0 0 0 0
26 29 1 0 0 0 0

Entry 10A Lewis acid = $CuCl_2$

Title Card Required

Created by GaussView 5.0.9
31 29 0 0 0 0 0 0 0 0 0 0 0
-0.4419 1.7893 -0.2955 N 0 0 0 0 0 0 0 0 0 0 0 0
-1.2568 2.9163 -0.7789 C 0 0 0 0 0 0 0 0 0 0 0 0
-0.5820 3.7139 -1.1042 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.8696 2.5908 -1.6295 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.9092 3.2858 0.0239 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.0233 0.6072 0.1257 C 0 0 0 0 0 0 0 0 0 0 0 0
-0.3697 -0.3548 0.5391 O 0 0 0 0 0 0 0 0 0 0 0 0
-2.3293 0.6603 0.0630 O 0 0 0 0 0 0 0 0 0 0 0 0

1.2816	1.9525	-0.2300	S	0	0	0	0	0	0	0	0	0	0	0	0
1.8758	0.7276	-0.8082	O	0	0	0	0	0	0	0	0	0	0	0	0
1.5894	3.2263	-0.8652	O	0	0	0	0	0	0	0	0	0	0	0	0
1.6644	2.0225	1.5114	C	0	0	0	0	0	0	0	0	0	0	0	0
1.1206	2.8728	1.9412	H	0	0	0	0	0	0	0	0	0	0	0	0
1.3994	1.0628	1.9723	H	0	0	0	0	0	0	0	0	0	0	0	0
2.7506	2.1802	1.5601	H	0	0	0	0	0	0	0	0	0	0	0	0
1.3679	-1.3050	-0.1331	Cu	0	0	0	0	0	0	0	0	0	0	0	0
2.5270	-1.4710	1.7312	Cl	0	0	0	0	0	0	0	0	0	0	0	0
0.7133	-2.2506	-1.9993	Cl	0	0	0	0	0	0	0	0	0	0	0	0
-3.2288	-0.4996	0.3771	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.6147	0.1125	0.1913	C	0	0	0	0	0	0	0	0	0	0	0	0
-5.3825	-0.6534	0.3747	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.7746	0.9413	0.8970	H	0	0	0	0	0	0	0	0	0	0	0	0
-4.7404	0.4924	-0.8333	H	0	0	0	0	0	0	0	0	0	0	0	0
-2.9682	-1.6094	-0.6391	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.1361	-1.2429	-1.6633	H	0	0	0	0	0	0	0	0	0	0	0	0
-1.9455	-2.0028	-0.5735	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.6711	-2.4356	-0.4534	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.0113	-0.9427	1.8233	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.0267	-1.4036	1.9672	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.1121	-0.0878	2.5095	H	0	0	0	0	0	0	0	0	0	0	0	0
-3.7845	-1.6804	2.0861	H	0	0	0	0	0	0	0	0	0	0	0	0

1	2	1	0	0	0	0
1	6	1	0	0	0	0
1	9	1	0	0	0	0
2	3	1	0	0	0	0
2	4	1	0	0	0	0
2	5	1	0	0	0	0
6	7	2	0	0	0	0
6	8	4	0	0	0	0
8	19	1	0	0	0	0
9	10	2	0	0	0	0
9	11	2	0	0	0	0
9	12	1	0	0	0	0
12	13	1	0	0	0	0
12	14	1	0	0	0	0
12	15	1	0	0	0	0
16	17	1	0	0	0	0
16	18	1	0	0	0	0
19	20	1	0	0	0	0
19	24	1	0	0	0	0
19	28	1	0	0	0	0
20	21	1	0	0	0	0
20	22	1	0	0	0	0
20	23	1	0	0	0	0

```
 24 25  1  0  0  0  0
 24 26  1  0  0  0  0
 24 27  1  0  0  0  0
 28 29  1  0  0  0  0
 28 30  1  0  0  0  0
 28 31  1  0  0  0  0
```

Entry 10B Lewis acid = $CuCl_2$

Title Card Required

Created by GaussView 5.0.9

```
 28 26  0  0  0  0  0  0  0  0  0  0    0
   -0.6447    1.9701    0.6074 N   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6452    2.9927    0.3150 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2736    3.6545   -0.4836 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5791    2.5269   -0.0104 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8386    3.6014    1.2128 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8856    0.6547    0.4975 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0125   -0.2183    0.6412 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1468    0.3356    0.2843 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.7532   -0.3631   -0.2161 Cu  0  0  0  0  0  0  0  0  0  0  0  0
    3.2069   -1.1409    1.1981 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    1.3272    0.4308   -2.2141 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -2.6355   -1.0434    0.0102 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.1306   -0.8169   -0.2121 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.6240   -1.7772   -0.4220 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.5954   -0.3745    0.6815 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.3007   -0.1448   -1.0664 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9729   -1.5831   -1.2572 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1150   -0.8856   -2.0963 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8973   -1.7478   -1.1220 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.4400   -2.5429   -1.5245 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3921   -1.9266    1.2344 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3216   -2.0956    1.4050 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.8291   -1.4669    2.1341 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.8804   -2.9006    1.0784 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.7002    2.4415    0.9228 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.2154    1.7252    1.5753 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.2919    2.5873    0.0031 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.6233    3.4009    1.4521 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  6  4  0  0  0  0
  1 25  1  0  0  0  0
  2  3  1  0  0  0  0
  2  4  1  0  0  0  0
```

```
 2  5  1  0  0  0  0
 6  7  2  0  0  0  0
 6  8  4  0  0  0  0
 8 12  1  0  0  0  0
 9 10  1  0  0  0  0
 9 11  1  0  0  0  0
12 13  1  0  0  0  0
12 17  1  0  0  0  0
12 21  1  0  0  0  0
13 14  1  0  0  0  0
13 15  1  0  0  0  0
13 16  1  0  0  0  0
17 18  1  0  0  0  0
17 19  1  0  0  0  0
17 20  1  0  0  0  0
21 22  1  0  0  0  0
21 23  1  0  0  0  0
21 24  1  0  0  0  0
25 26  1  0  0  0  0
25 27  1  0  0  0  0
25 28  1  0  0  0  0
```

Entry 11A Lewis acid = $FeCl_3$

itle Card Required

Created by GaussView 5.0.9

```
 32 30  0  0  0  0  0  0  0  0  0    0
    0.9818    1.3902    0.4829 N   0  0  0  0  0  0  0  0  0  0  0  0
    1.0509    1.4812    1.9539 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.5309    2.3890    2.2767 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.5850    0.6024    2.4227 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.1057    1.5431    2.2406 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.8327    0.5513   -0.2726 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.7144    0.4310   -1.4729 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.7298   -0.0099    0.5134 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.4030    2.0019   -0.2793 S   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1905    0.8416   -0.8404 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0810    2.8545    0.6859 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.1248    2.9419   -1.6947 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.7434    3.7664   -1.3189 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.6738    2.2759   -2.3673 H   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8049    3.3151   -2.1456 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.1083   -0.7584   -0.0109 Fe  0  0  0  0  0  0  0  0  0  0  0  0
   -0.5526   -2.3124    0.2843 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -2.8912   -0.0073    1.9169 Cl  0  0  0  0  0  0  0  0  0  0  0  0
```

-3.6770	-1.3036	-1.4591	Cl	0	0	0	0	0	0	0	0	0	0	0	0
3.8208	-0.8869	-0.0028	C	0	0	0	0	0	0	0	0	0	0	0	0
3.2121	-2.1214	-0.6664	C	0	0	0	0	0	0	0	0	0	0	0	0
2.6639	-1.8591	-1.5799	H	0	0	0	0	0	0	0	0	0	0	0	0
4.0194	-2.8214	-0.9306	H	0	0	0	0	0	0	0	0	0	0	0	0
2.5231	-2.6308	0.0229	H	0	0	0	0	0	0	0	0	0	0	0	0
4.5717	-1.2592	1.2737	C	0	0	0	0	0	0	0	0	0	0	0	0
5.4166	-1.9195	1.0290	H	0	0	0	0	0	0	0	0	0	0	0	0
4.9656	-0.3607	1.7720	H	0	0	0	0	0	0	0	0	0	0	0	0
3.9089	-1.7877	1.9748	H	0	0	0	0	0	0	0	0	0	0	0	0
4.7062	-0.0802	-0.9524	C	0	0	0	0	0	0	0	0	0	0	0	0
4.1628	0.2073	-1.8616	H	0	0	0	0	0	0	0	0	0	0	0	0
5.0823	0.8274	-0.4557	H	0	0	0	0	0	0	0	0	0	0	0	0
5.5727	-0.6925	-1.2448	H	0	0	0	0	0	0	0	0	0	0	0	0

1	2	1	0	0	0	0
1	6	1	0	0	0	0
1	9	1	0	0	0	0
2	3	1	0	0	0	0
2	4	1	0	0	0	0
2	5	1	0	0	0	0
6	7	2	0	0	0	0
6	8	4	0	0	0	0
8	20	1	0	0	0	0
9	10	4	0	0	0	0
9	11	2	0	0	0	0
9	12	1	0	0	0	0
12	13	1	0	0	0	0
12	14	1	0	0	0	0
12	15	1	0	0	0	0
16	17	1	0	0	0	0
16	18	1	0	0	0	0
16	19	1	0	0	0	0
20	21	1	0	0	0	0
20	25	1	0	0	0	0
20	29	1	0	0	0	0
21	22	1	0	0	0	0
21	23	1	0	0	0	0
21	24	1	0	0	0	0
25	26	1	0	0	0	0
25	27	1	0	0	0	0
25	28	1	0	0	0	0
29	30	1	0	0	0	0
29	31	1	0	0	0	0
29	32	1	0	0	0	0

Entry 12A Lewis acid = $InCl_3$

Title Card Required

Created by GaussView 5.0.9
```
 32 31  0  0  0  0  0  0  0  0  0    0
  -1.3838    1.5333   -0.3985 N   0  0  0  0  0  0  0  0  0  0  0  0
  -1.6218    1.8226   -1.8244 C   0  0  0  0  0  0  0  0  0  0  0  0
  -1.0714    2.7293   -2.0951 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.2841    0.9833   -2.4482 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.6950    1.9900   -1.9705 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.1232    0.5613    0.3099 C   0  0  0  0  0  0  0  0  0  0  0  0
  -1.9233    0.3306    1.4832 O   0  0  0  0  0  0  0  0  0  0  0  0
  -3.0184    0.0091   -0.4846 O   0  0  0  0  0  0  0  0  0  0  0  0
   0.0006    2.1655    0.3466 S   0  0  0  0  0  0  0  0  0  0  0  0
   0.8431    1.0272    0.8613 O   0  0  0  0  0  0  0  0  0  0  0  0
   0.6255    3.0702   -0.6086 O   0  0  0  0  0  0  0  0  0  0  0  0
  -0.5455    3.0356    1.7995 C   0  0  0  0  0  0  0  0  0  0  0  0
  -1.1813    3.8622    1.4580 H   0  0  0  0  0  0  0  0  0  0  0  0
  -1.0840    2.3251    2.4360 H   0  0  0  0  0  0  0  0  0  0  0  0
   0.3695    3.4067    2.2804 H   0  0  0  0  0  0  0  0  0  0  0  0
   2.3214   -2.0144    1.8504 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   0.3847   -1.4483   -1.6482 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   3.8976    0.3937   -0.9737 Cl  0  0  0  0  0  0  0  0  0  0  0  0
  -3.9431   -1.0676   -0.0302 C   0  0  0  0  0  0  0  0  0  0  0  0
  -4.8720   -0.5109    1.0485 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.6193   -1.2754    1.3098 H   0  0  0  0  0  0  0  0  0  0  0  0
  -4.3174   -0.2434    1.9572 H   0  0  0  0  0  0  0  0  0  0  0  0
  -5.4071    0.3774    0.6791 H   0  0  0  0  0  0  0  0  0  0  0  0
  -3.1279   -2.2687    0.4509 C   0  0  0  0  0  0  0  0  0  0  0  0
  -3.8049   -3.1211    0.6128 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.3830   -2.5556   -0.3066 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.6077   -2.0532    1.3927 H   0  0  0  0  0  0  0  0  0  0  0  0
  -4.7119   -1.3988   -1.3075 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.4519   -2.1861   -1.1018 H   0  0  0  0  0  0  0  0  0  0  0  0
  -5.2429   -0.5119   -1.6844 H   0  0  0  0  0  0  0  0  0  0  0  0
  -4.0284   -1.7584   -2.0910 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.9730   -0.6472   -0.0563 In  0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  6  1  0  0  0  0
 1  9  1  0  0  0  0
 2  3  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 6  7  2  0  0  0  0
 6  8  4  0  0  0  0
 8 19  1  0  0  0  0
```

```
 9 10  4  0  0  0  0
 9 11  2  0  0  0  0
 9 12  1  0  0  0  0
10 32  1  0  0  0  0
12 13  1  0  0  0  0
12 14  1  0  0  0  0
12 15  1  0  0  0  0
16 32  1  0  0  0  0
17 32  1  0  0  0  0
18 32  1  0  0  0  0
19 20  1  0  0  0  0
19 24  1  0  0  0  0
19 28  1  0  0  0  0
20 21  1  0  0  0  0
20 22  1  0  0  0  0
20 23  1  0  0  0  0
24 25  1  0  0  0  0
24 26  1  0  0  0  0
24 27  1  0  0  0  0
28 29  1  0  0  0  0
28 30  1  0  0  0  0
28 31  1  0  0  0  0
```

Entry 13A Lewis acid = $RuCl_3$

Title Card Required

Created by GaussView 5.0.9

```
 32 28  0  0  0  0  0  0  0  0  0  0    0
   -1.3322    1.4649   -0.4767 N   0  0  0  0  0  0  0  0  0  0  0  0
   -1.5392    1.6546   -1.9233 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9482    2.5156   -2.2515 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2230    0.7573   -2.4734 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6023    1.8499   -2.1067 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.0805    0.5364    0.2747 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8888    0.3566    1.4587 O   0  0  0  0  0  0  0  0  0  0  0  0
   -2.9808   -0.0426   -0.4973 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.0093    2.1909    0.2702 S   0  0  0  0  0  0  0  0  0  0  0  0
    0.8737    1.1185    0.8699 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.6249    3.0650   -0.7212 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6186    3.1290    1.6473 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2766    3.9062    1.2390 H   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1455    2.4382    2.3145 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.2662    3.5671    2.1286 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.5255   -1.7155   -1.5211 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    3.9172    0.2408   -1.1070 Cl  0  0  0  0  0  0  0  0  0  0  0  0
```

```
  2.5315   -1.7972    1.9645 Cl  0  0  0  0  0  0  0  0  0  0  0  0
 -3.9170   -1.0878    0.0003 C   0  0  0  0  0  0  0  0  0  0  0  0
 -3.1105   -2.2916    0.4887 C   0  0  0  0  0  0  0  0  0  0  0  0
 -2.5633   -2.0619    1.4120 H   0  0  0  0  0  0  0  0  0  0  0  0
 -3.7954   -3.1296    0.6880 H   0  0  0  0  0  0  0  0  0  0  0  0
 -2.3893   -2.6073   -0.2803 H   0  0  0  0  0  0  0  0  0  0  0  0
 -4.7212   -1.4306   -1.2520 C   0  0  0  0  0  0  0  0  0  0  0  0
 -5.4699   -2.2003   -1.0135 H   0  0  0  0  0  0  0  0  0  0  0  0
 -5.2458   -0.5416   -1.6330 H   0  0  0  0  0  0  0  0  0  0  0  0
 -4.0635   -1.8170   -2.0447 H   0  0  0  0  0  0  0  0  0  0  0  0
 -4.8143   -0.4941    1.0866 C   0  0  0  0  0  0  0  0  0  0  0  0
 -4.2391   -0.2256    1.9818 H   0  0  0  0  0  0  0  0  0  0  0  0
 -5.3354    0.4007    0.7127 H   0  0  0  0  0  0  0  0  0  0  0  0
 -5.5745   -1.2374    1.3707 H   0  0  0  0  0  0  0  0  0  0  0  0
  1.9999   -0.6222   -0.0128 Ru  0  0  0  0  0  0  0  0  0  0  0  0
 1  2  1  0  0  0  0
 1  6  1  0  0  0  0
 1  9  1  0  0  0  0
 2  3  1  0  0  0  0
 2  4  1  0  0  0  0
 2  5  1  0  0  0  0
 6  7  2  0  0  0  0
 6  8  4  0  0  0  0
 8 19  1  0  0  0  0
 9 10  2  0  0  0  0
 9 11  2  0  0  0  0
 9 12  1  0  0  0  0
12 13  1  0  0  0  0
12 14  1  0  0  0  0
12 15  1  0  0  0  0
18 32  1  0  0  0  0
19 20  1  0  0  0  0
19 24  1  0  0  0  0
19 28  1  0  0  0  0
20 21  1  0  0  0  0
20 22  1  0  0  0  0
20 23  1  0  0  0  0
24 25  1  0  0  0  0
24 26  1  0  0  0  0
24 27  1  0  0  0  0
28 29  1  0  0  0  0
28 30  1  0  0  0  0
28 31  1  0  0  0  0
```