**Supporting information**

# A Two-steps Telescoped Continuous Flow Switchable Process Leading to Nitriles, Diaziridine or Hydrazine Derivatives

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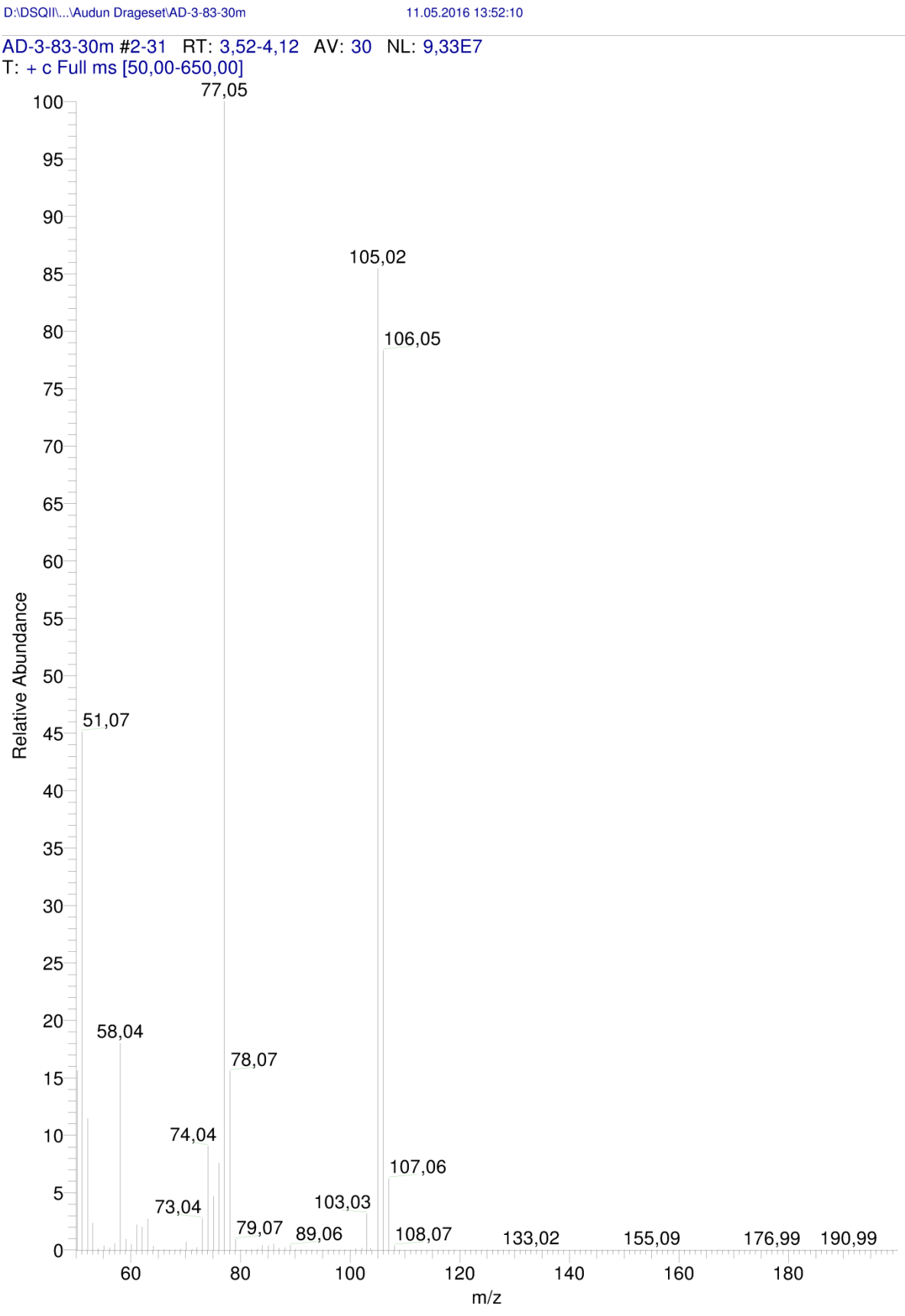
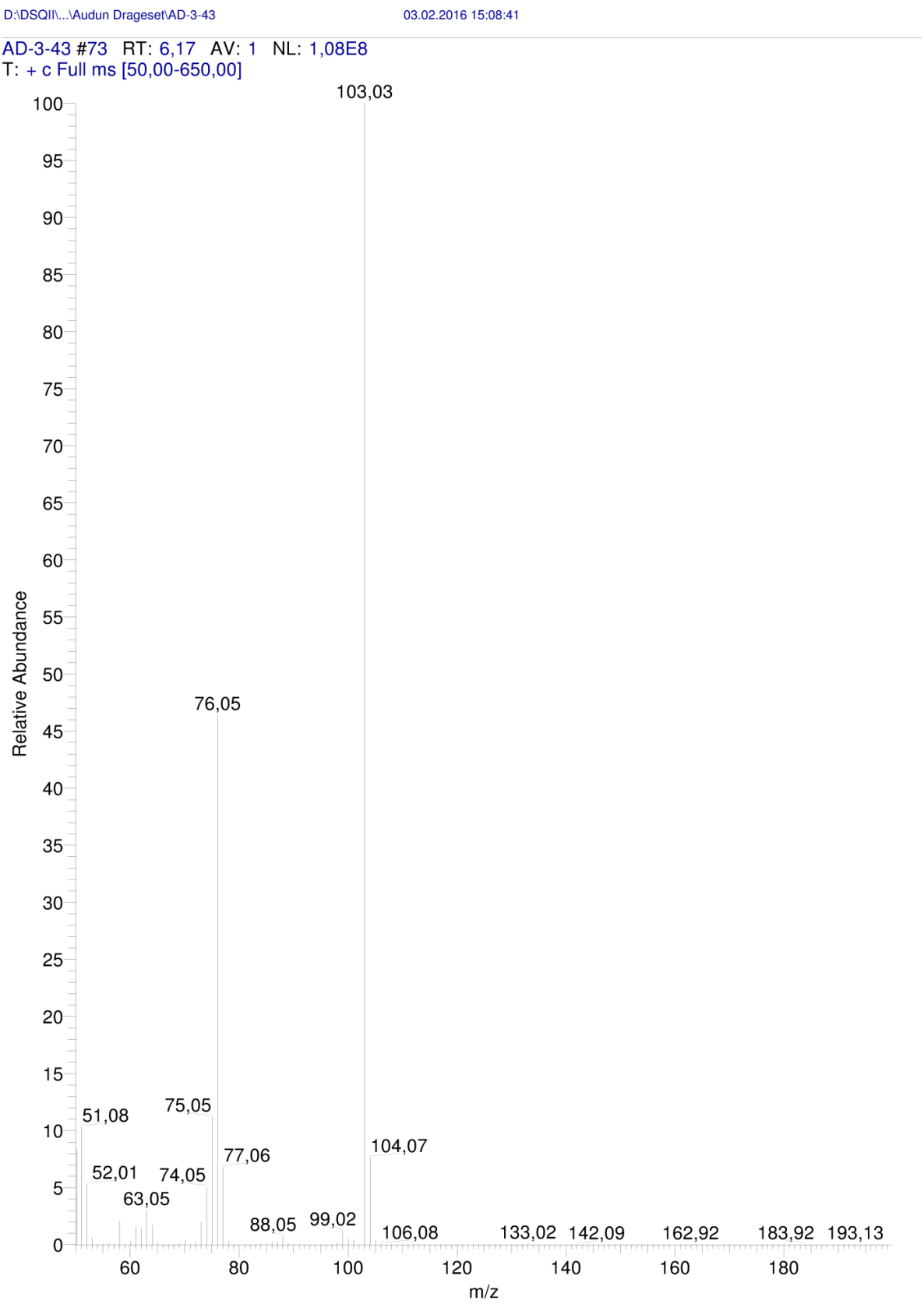
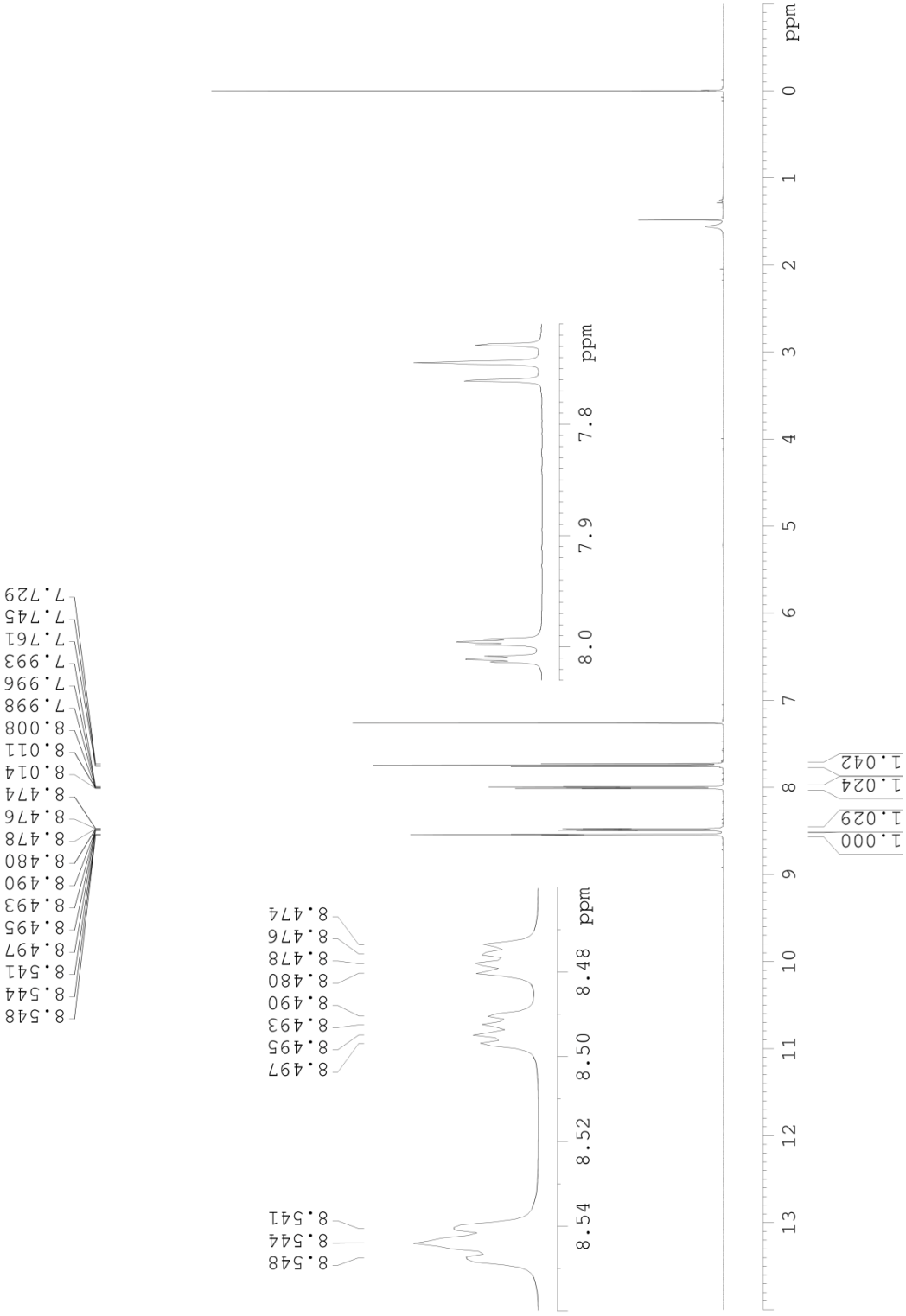
## Benzaldehyde (2a): GC-MS



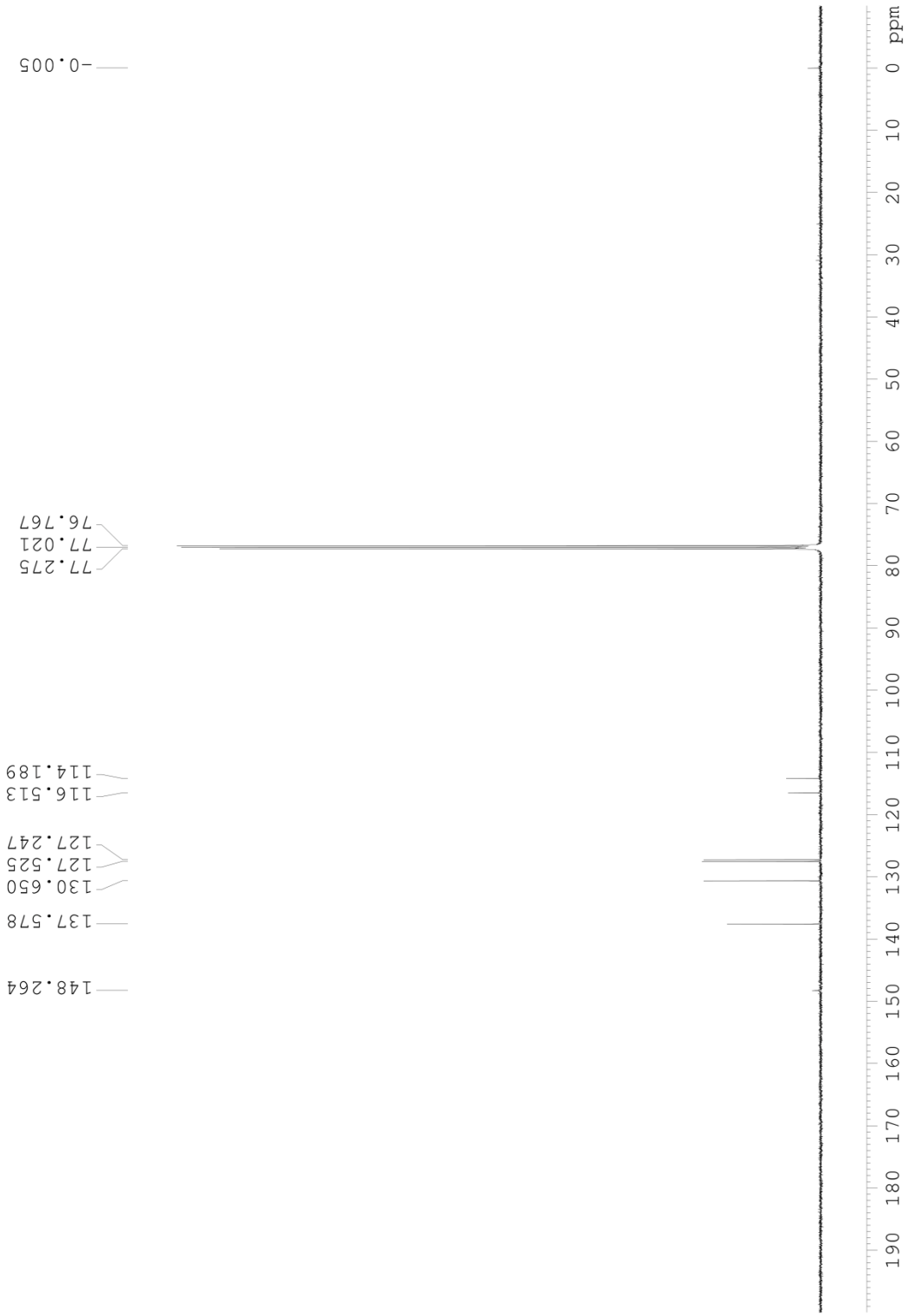
## Benzonitrile (3a): GC-MS



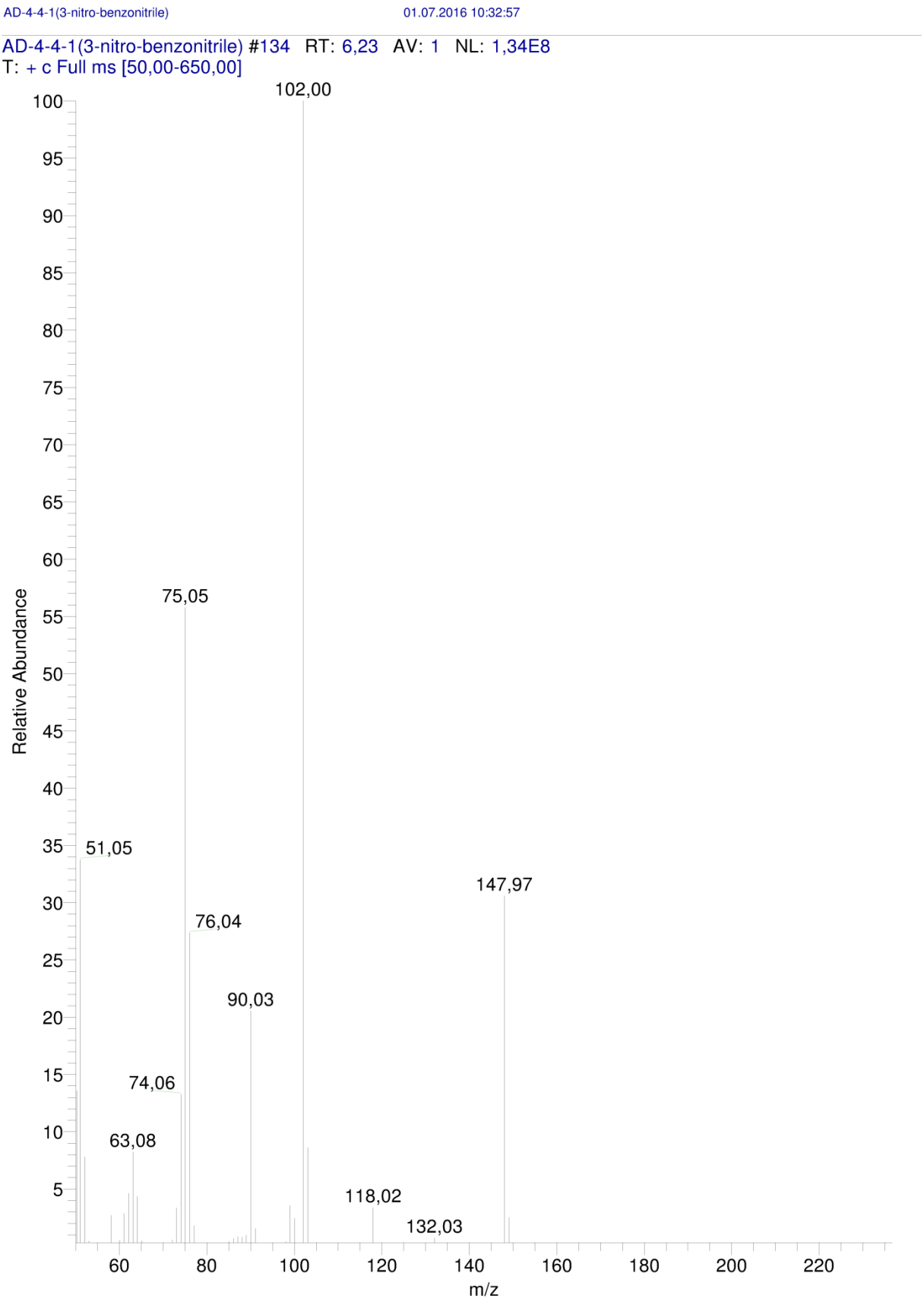
## 3-nitrobenzonitrile (3b): $^{1}$H-NMR in $CDCl_3$



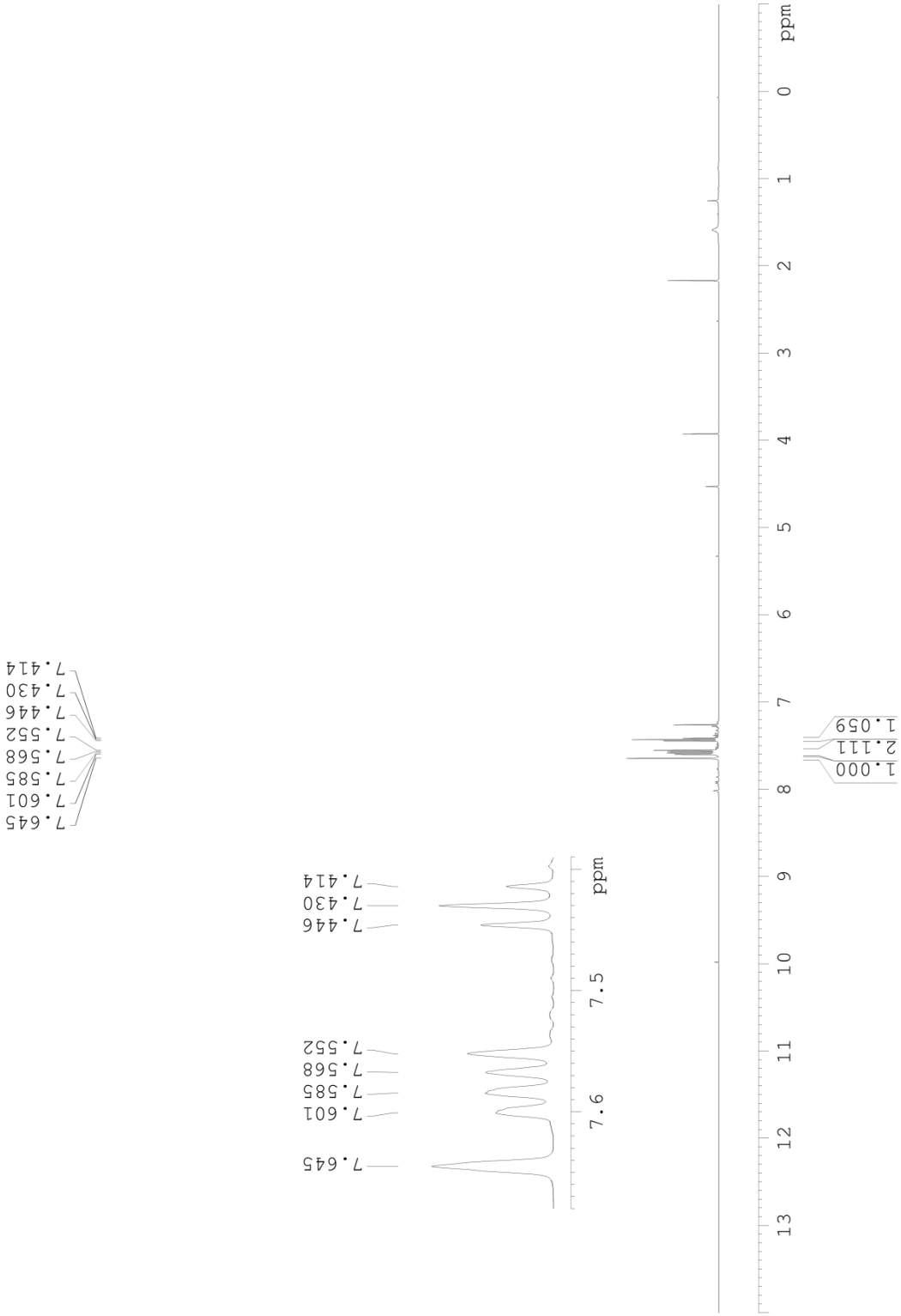
## 3-nitrobenzonitrile (3b): $^{13}$C-NMR in $CDCl_3$



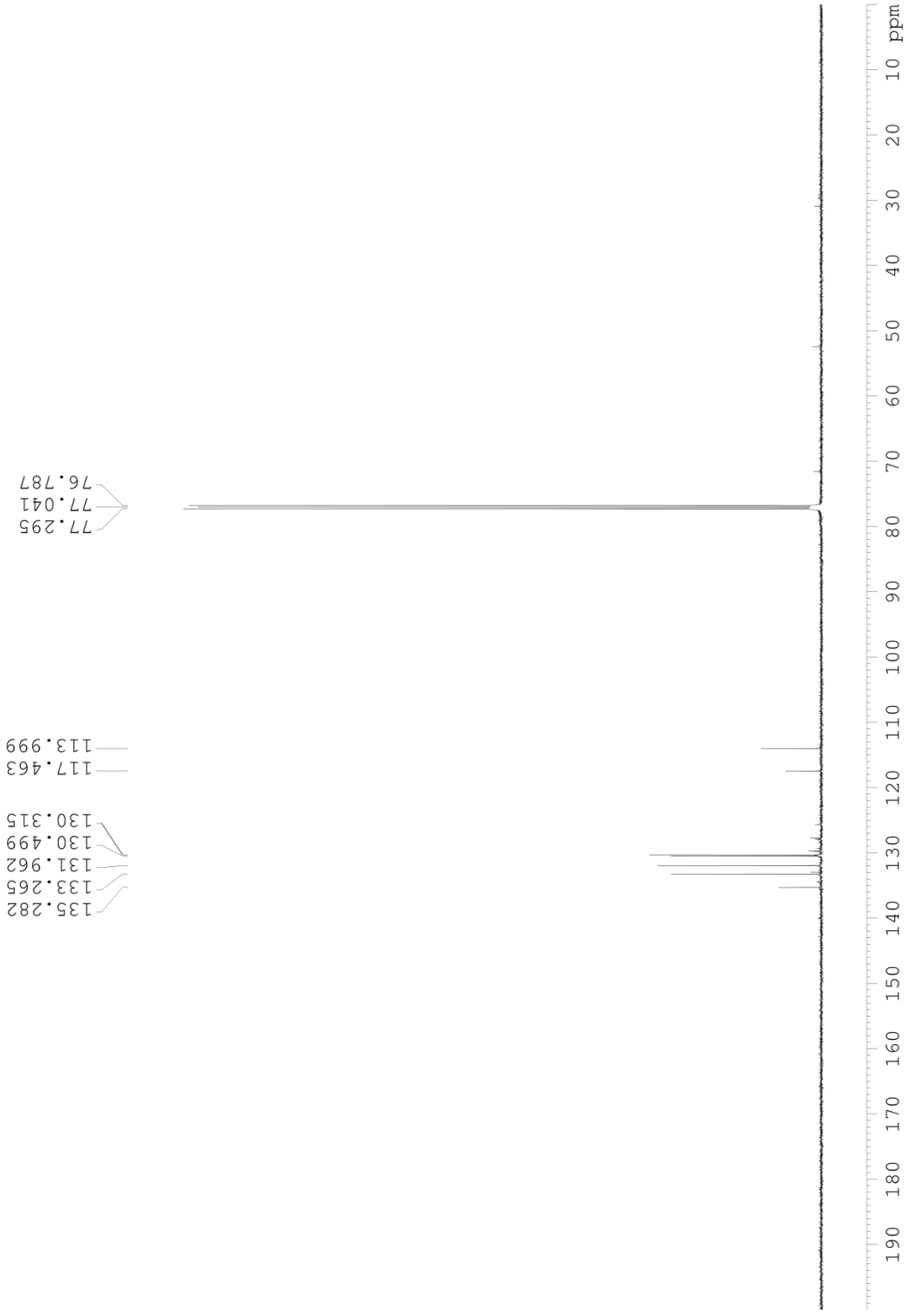
## 3-nitrobenzonitrile (3b): GC-MS



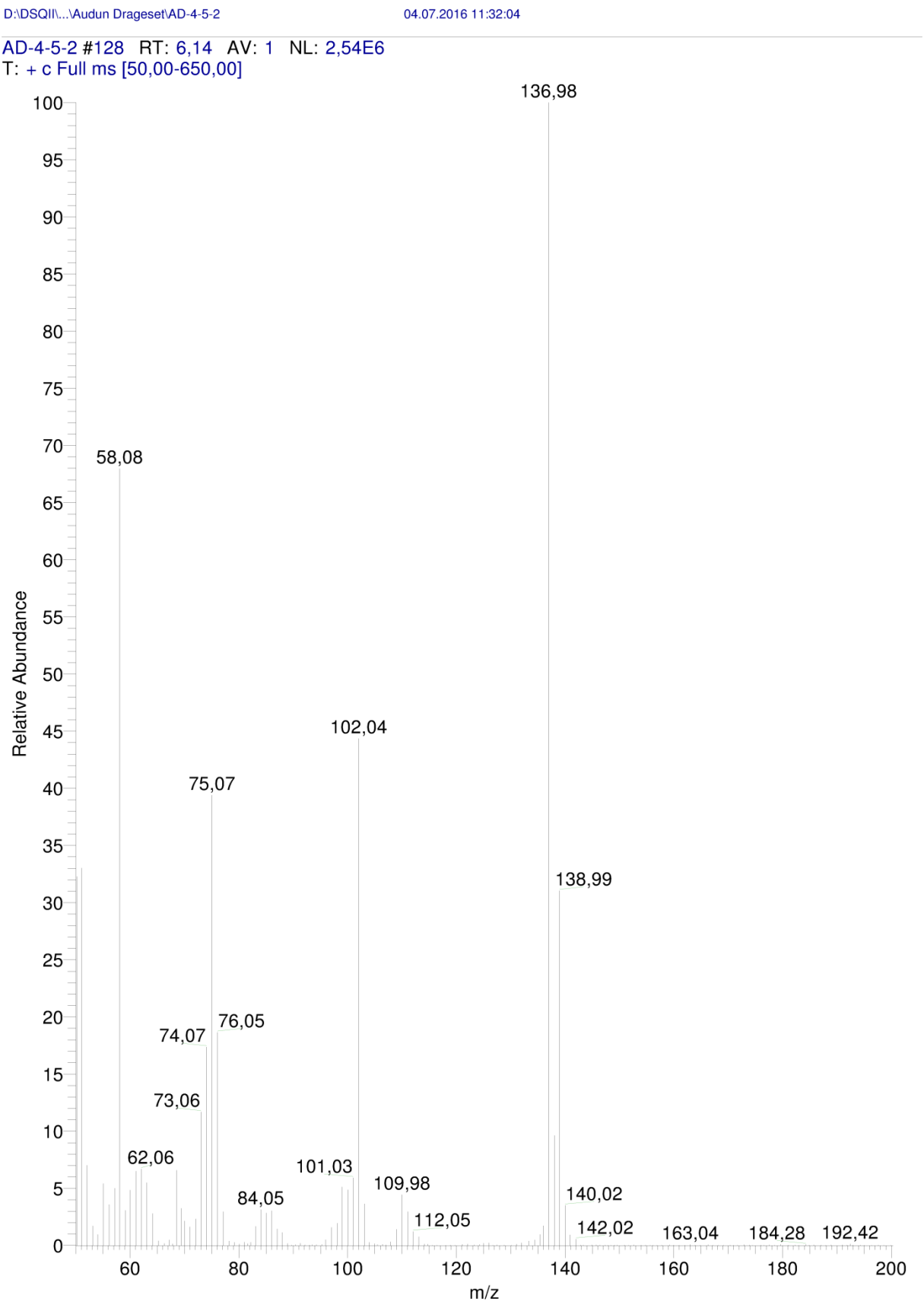
## 3-Chlorobenzonitrile (3c): $^{1}$H-NMR in $CDCl_3$



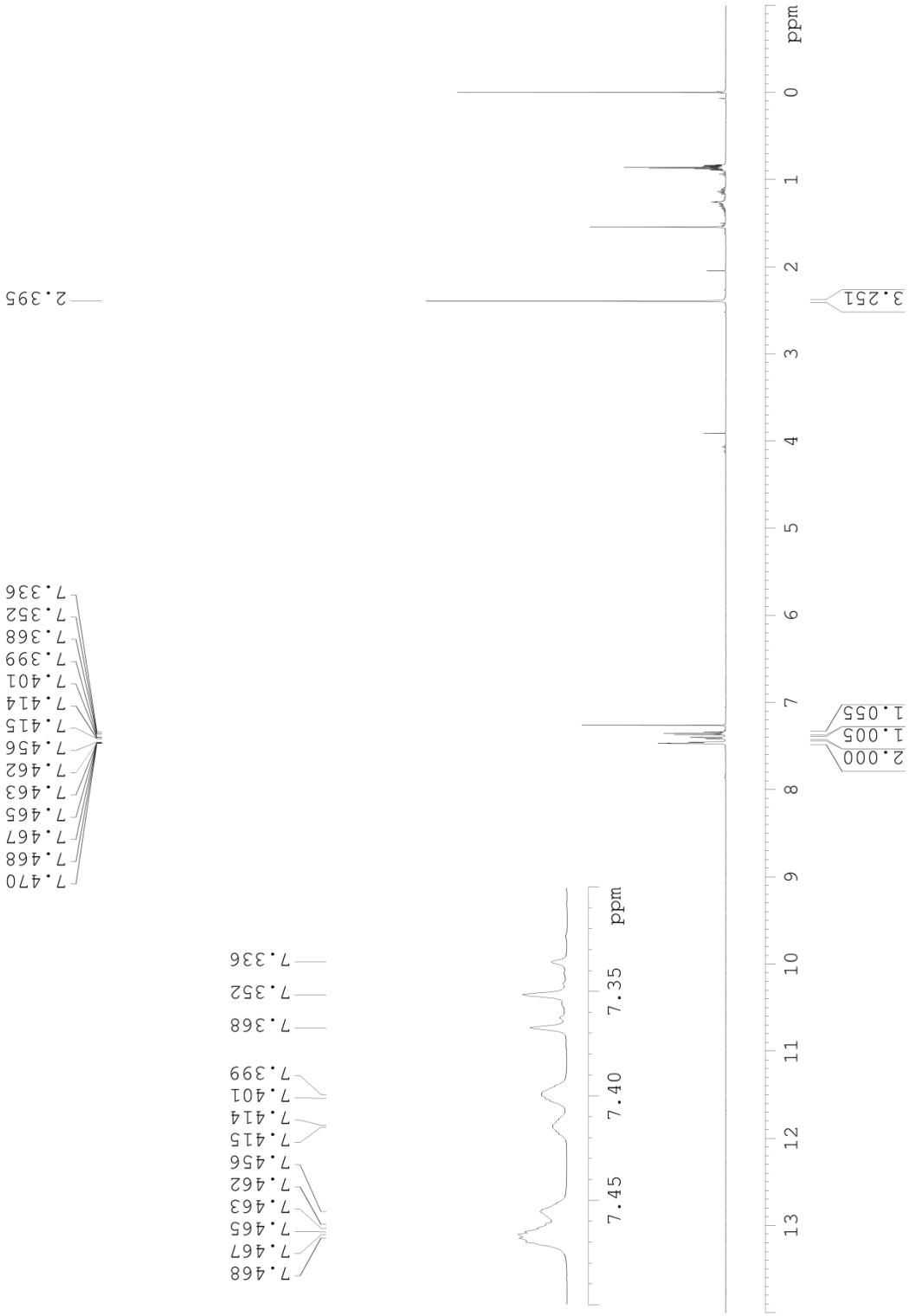
## 3-Chlorobenzonitrile (3c): $^{13}$C-NMR in $CDCl_3$



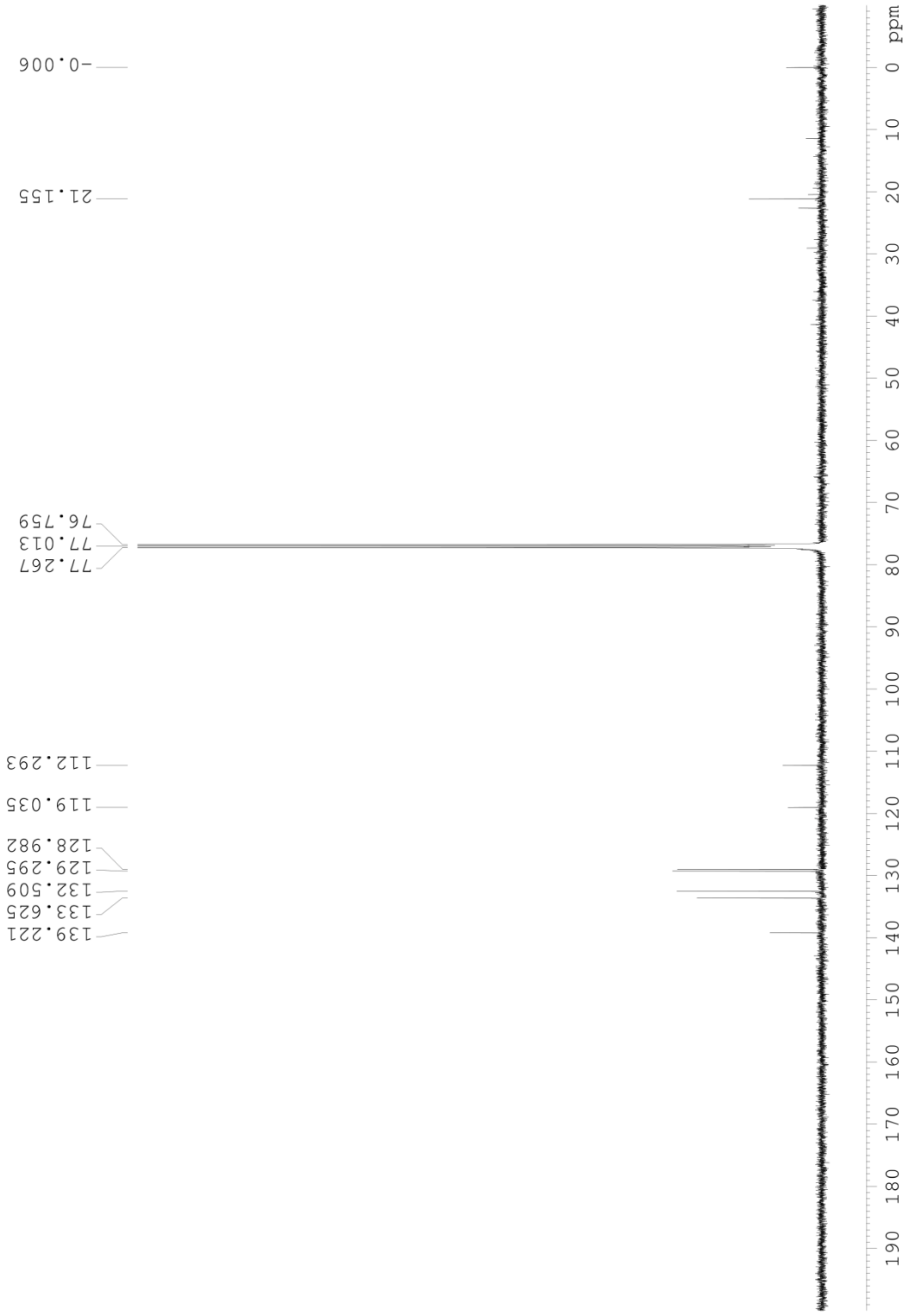
## 3-Chlorobenzonitrile (3c): GC-MS



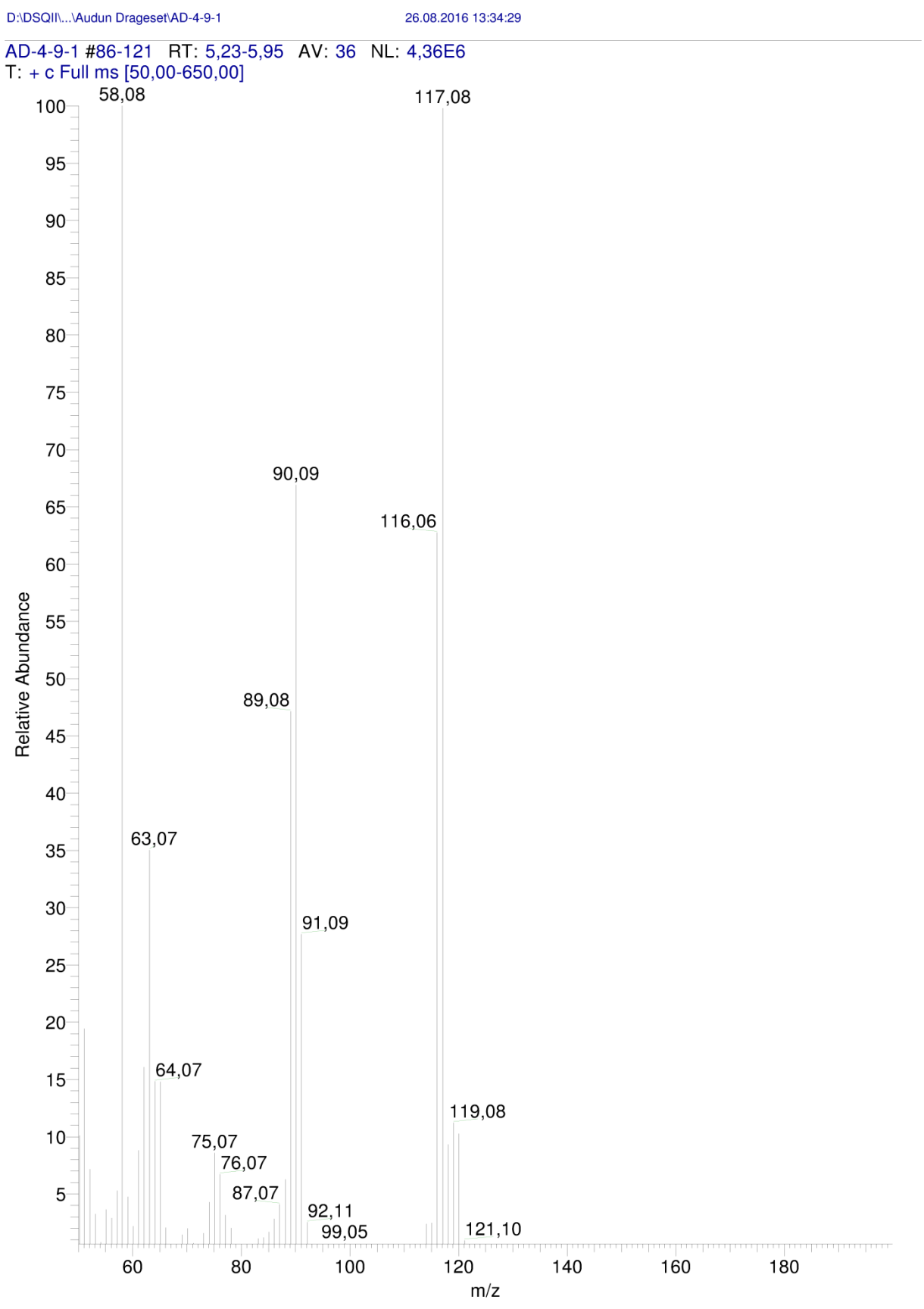
## 3-methylbenzonitrile (3d): $^{1}$H-NMR in $CDCl_3$



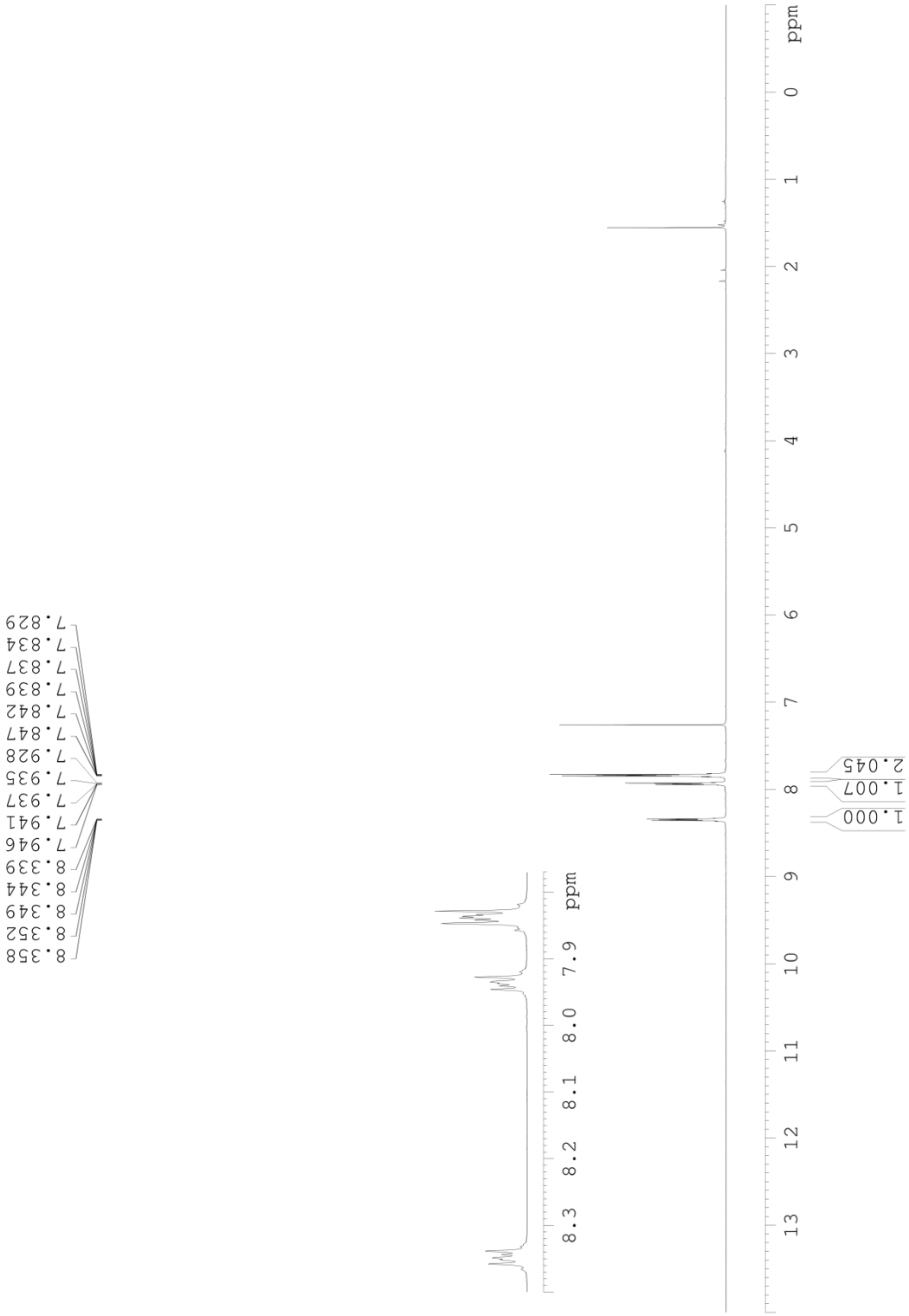
## 3-methylbenzonitrile (3d): $^{13}$C-NMR in $CDCl_3$



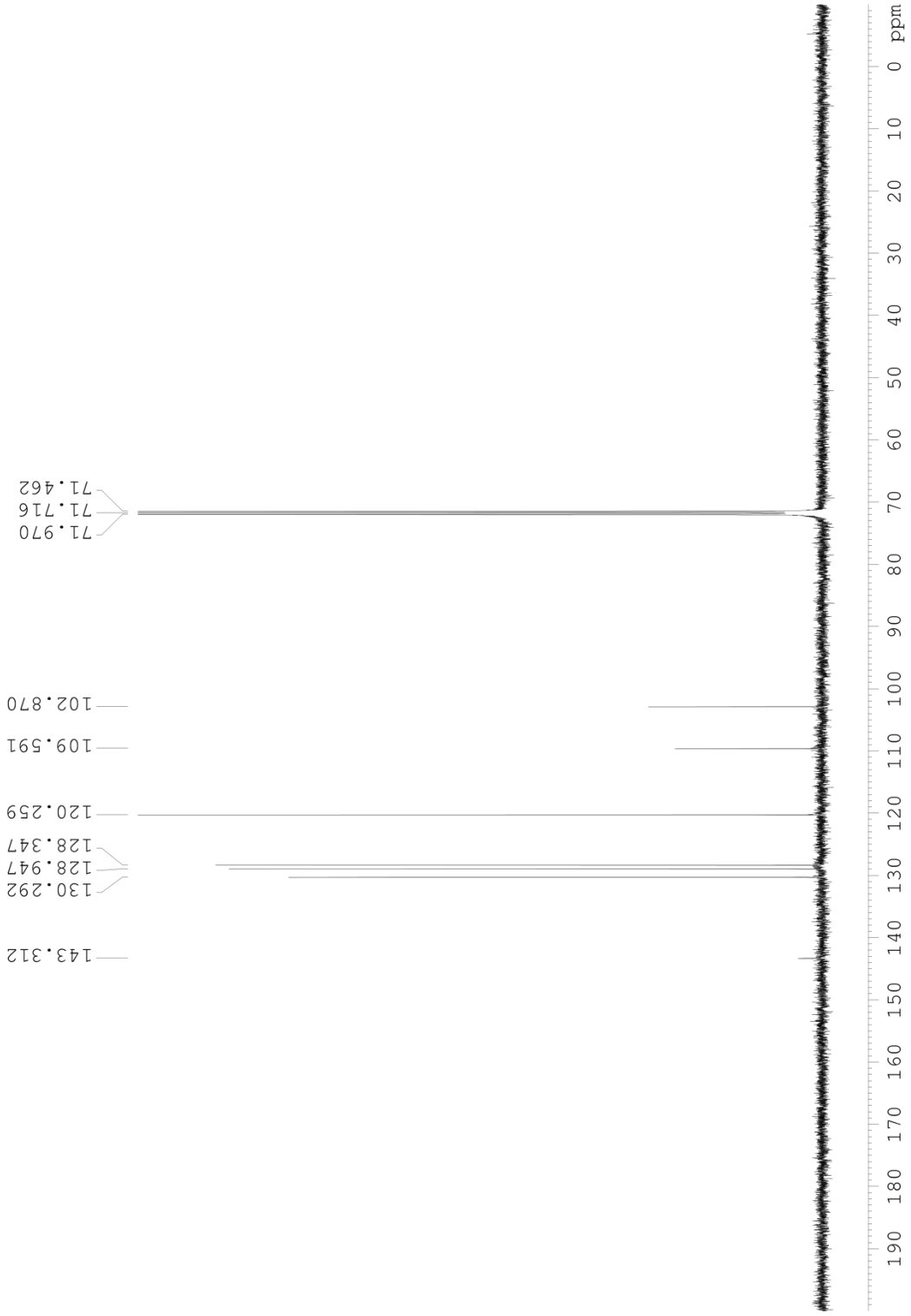
## 3-methylbenzonitrile (3d): GC-MS



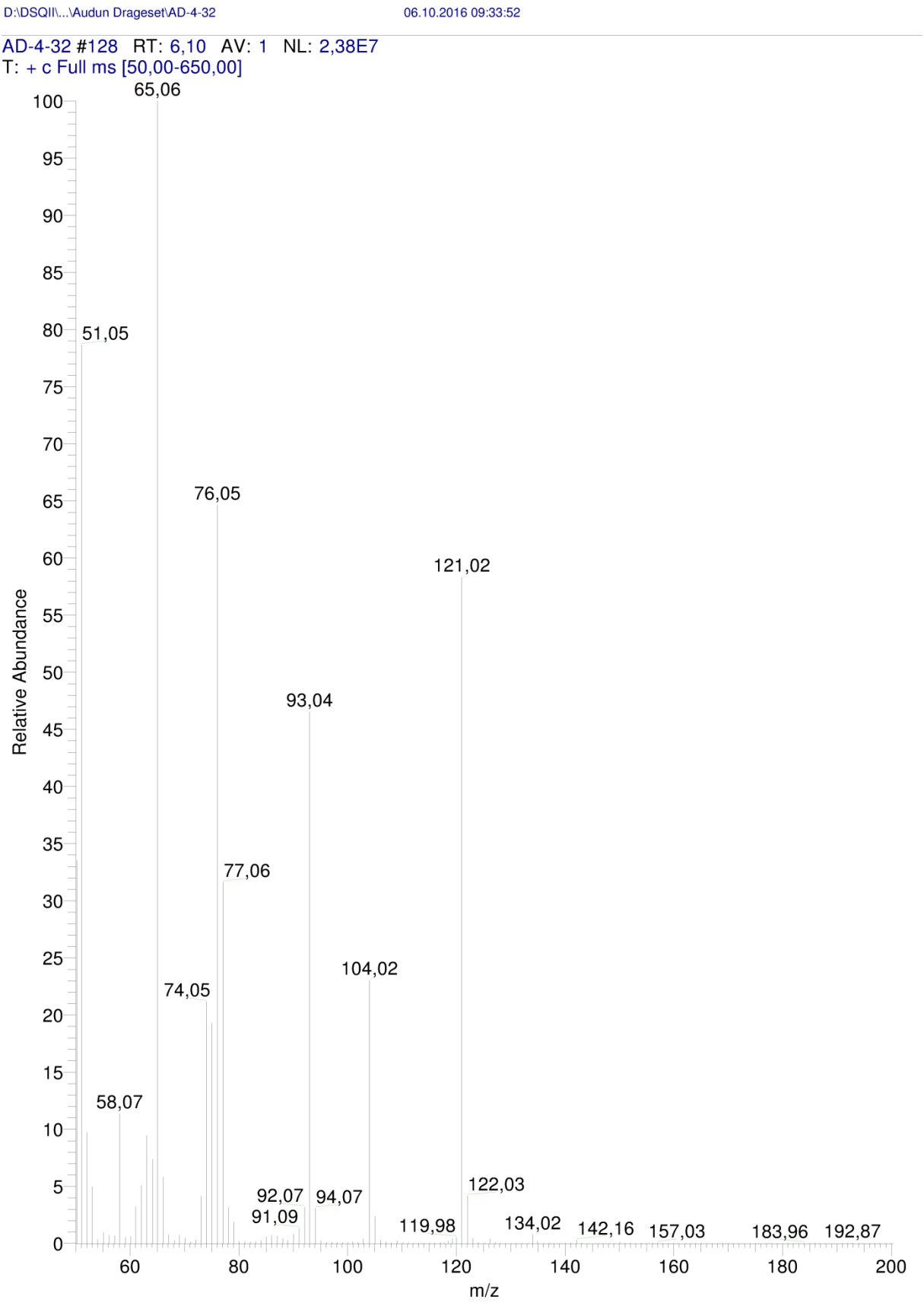
## 2-nitrobenzonitrile (3f): $^{1}$H-NMR in $CDCl_3$



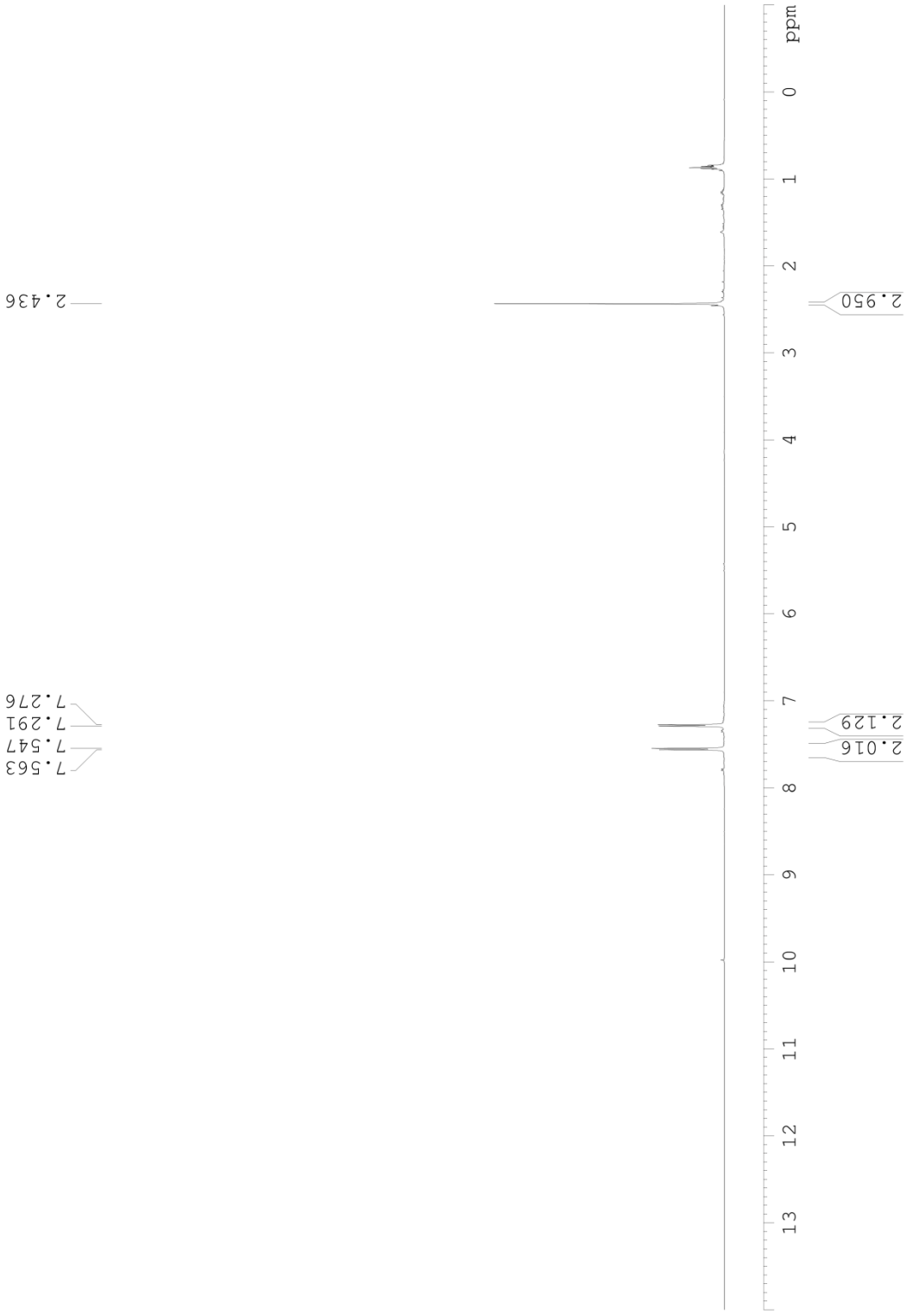
## 2-nitrobenzonitrile (3f): $^{13}$C-NMR in $CDCl_3$



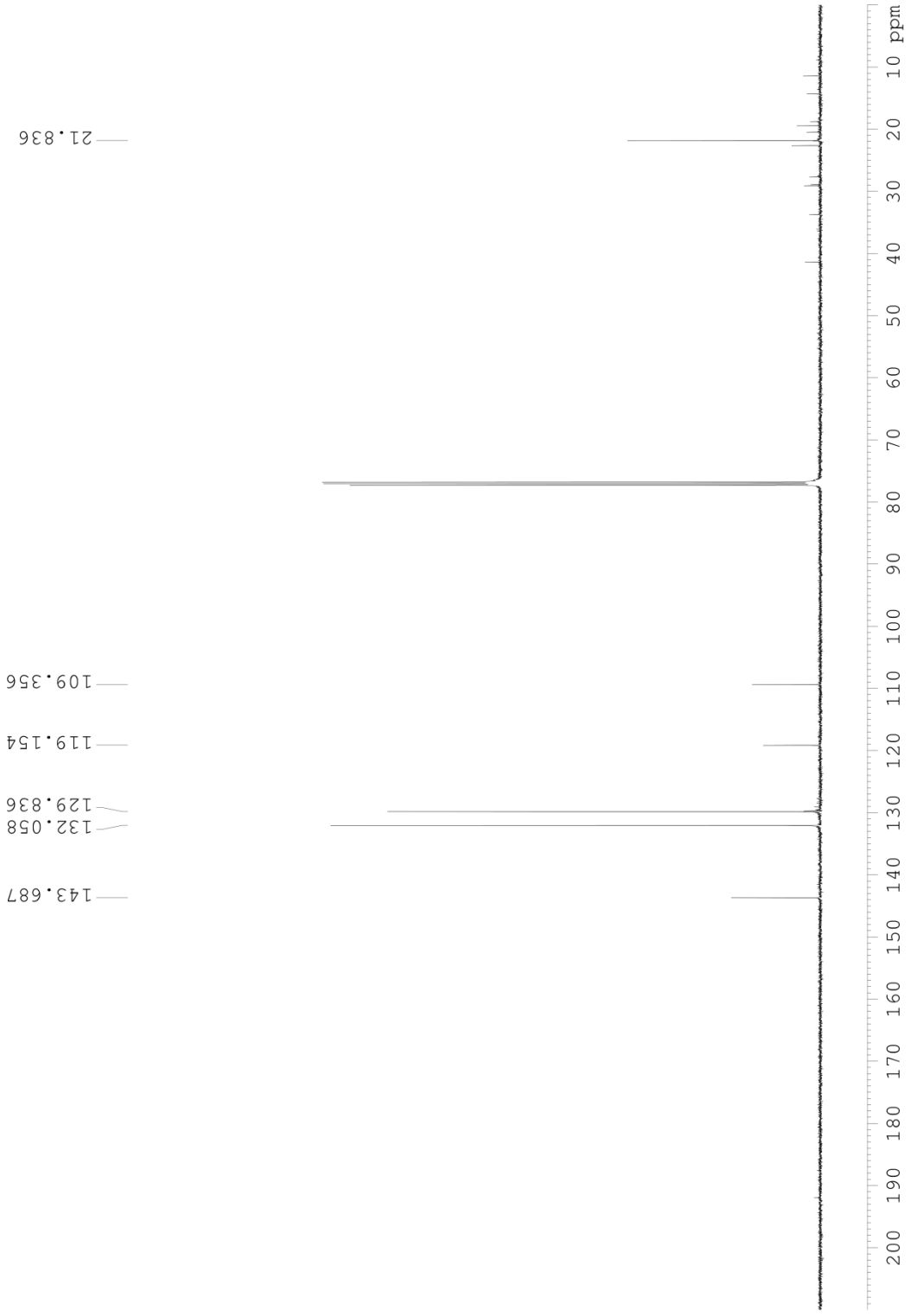
## 2-nitrobenzonitrile (3f): GC-MS



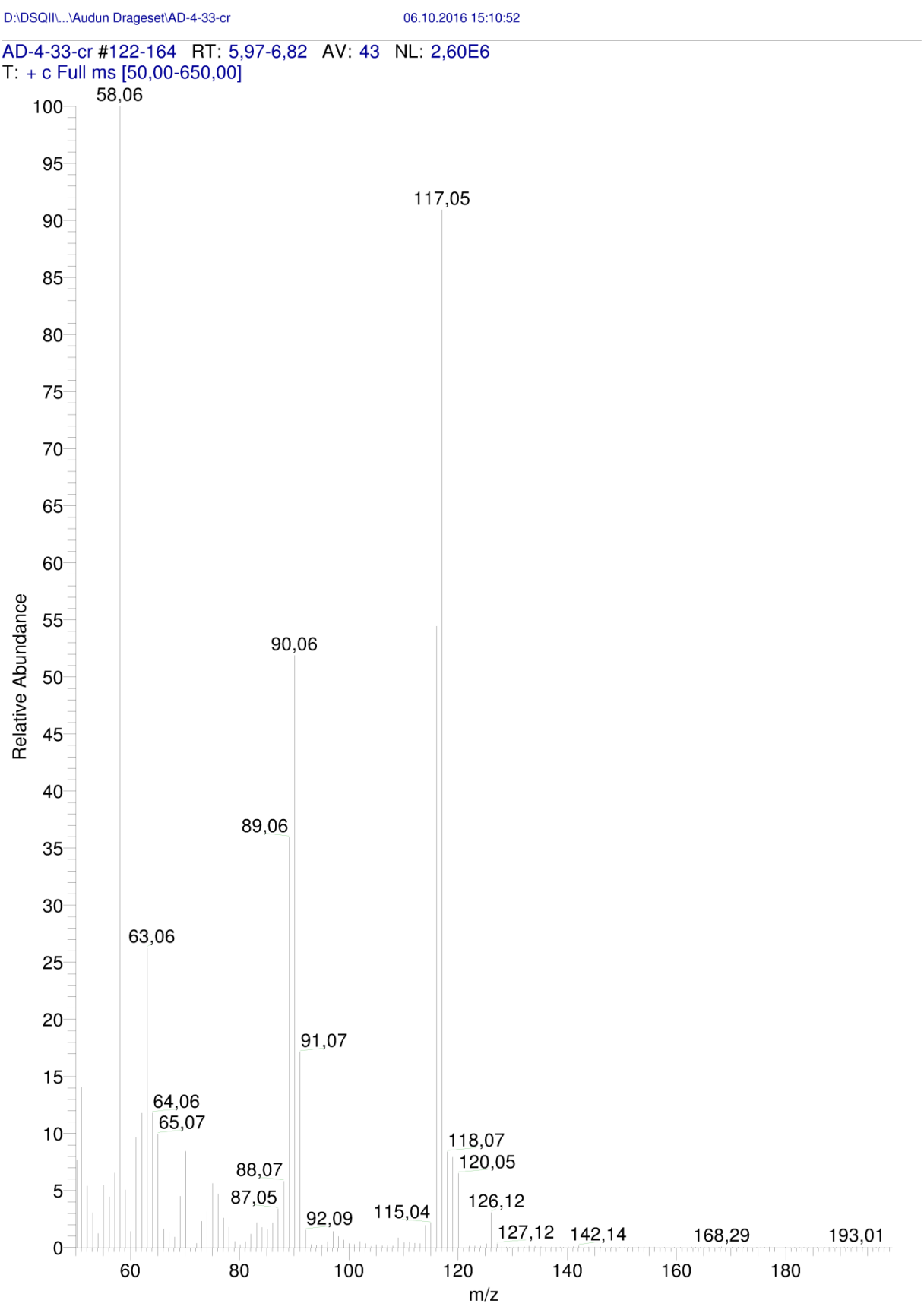
## 4-methylbenzonitrile (3g): $^{1}$H-NMR in $CDCl_3$



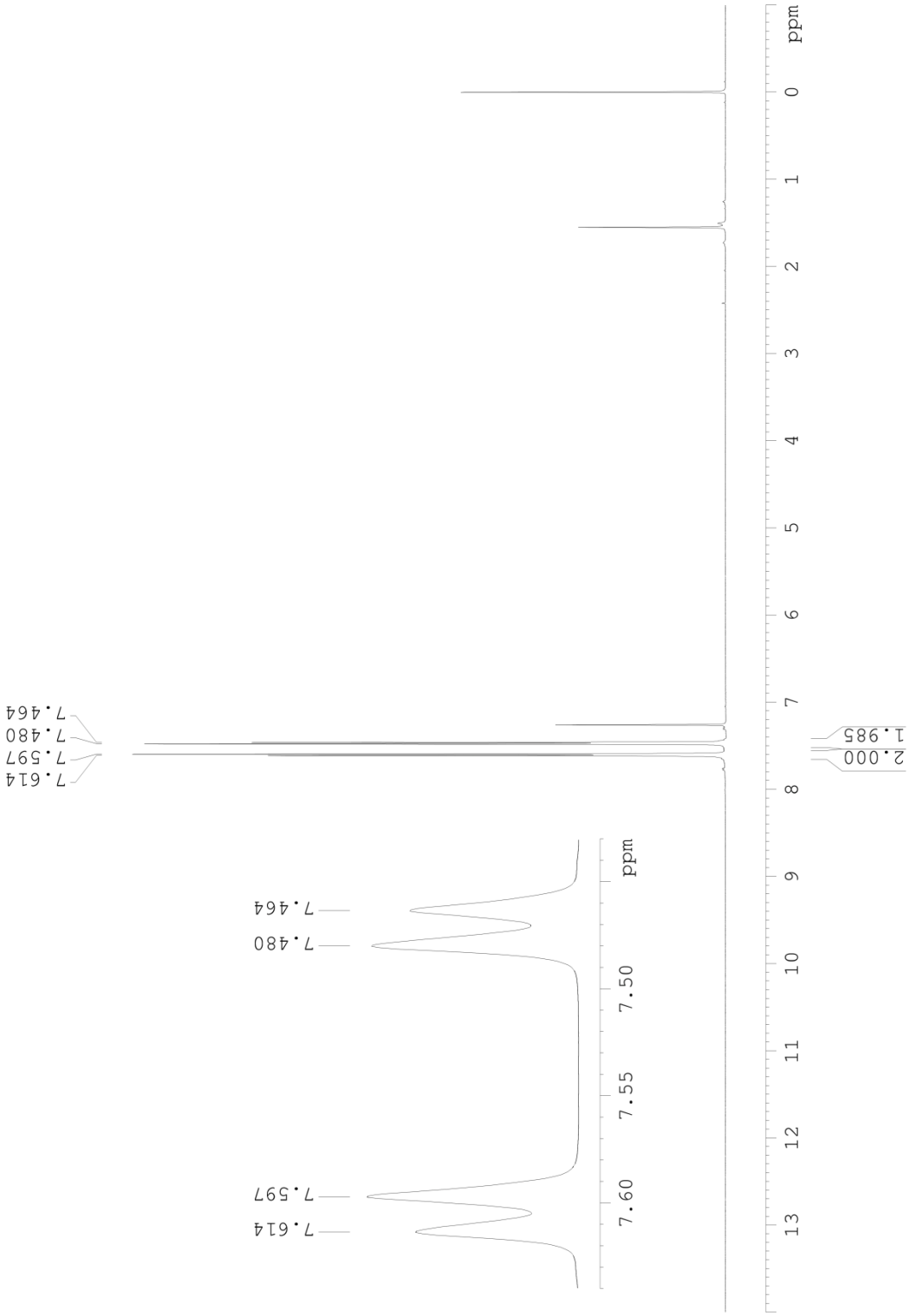
## 4-methylbenzonitrile (3g): $^{13}$C-NMR in $CDCl_3$



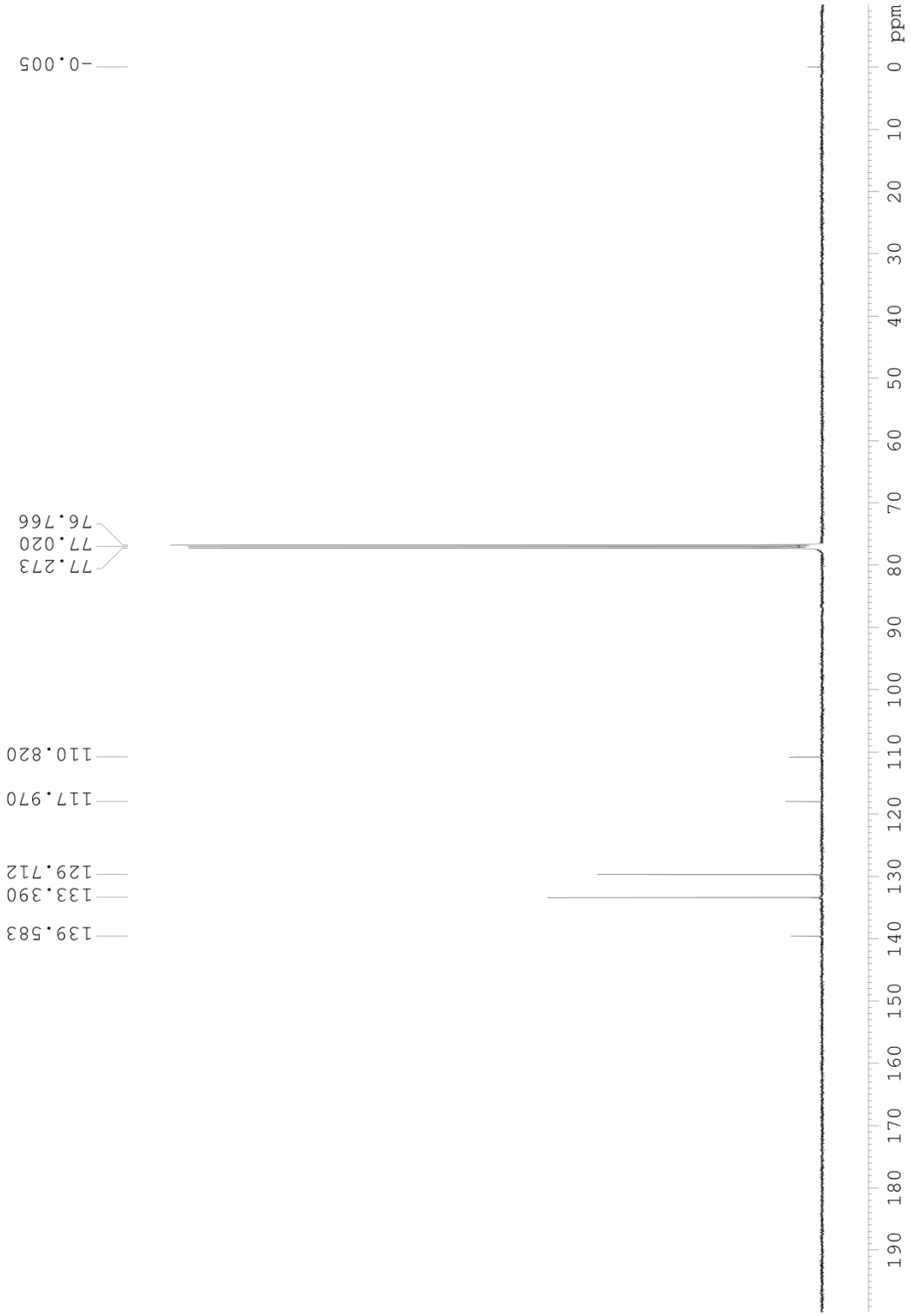
## 4-methylbenzonitrile (3g): GC-MS



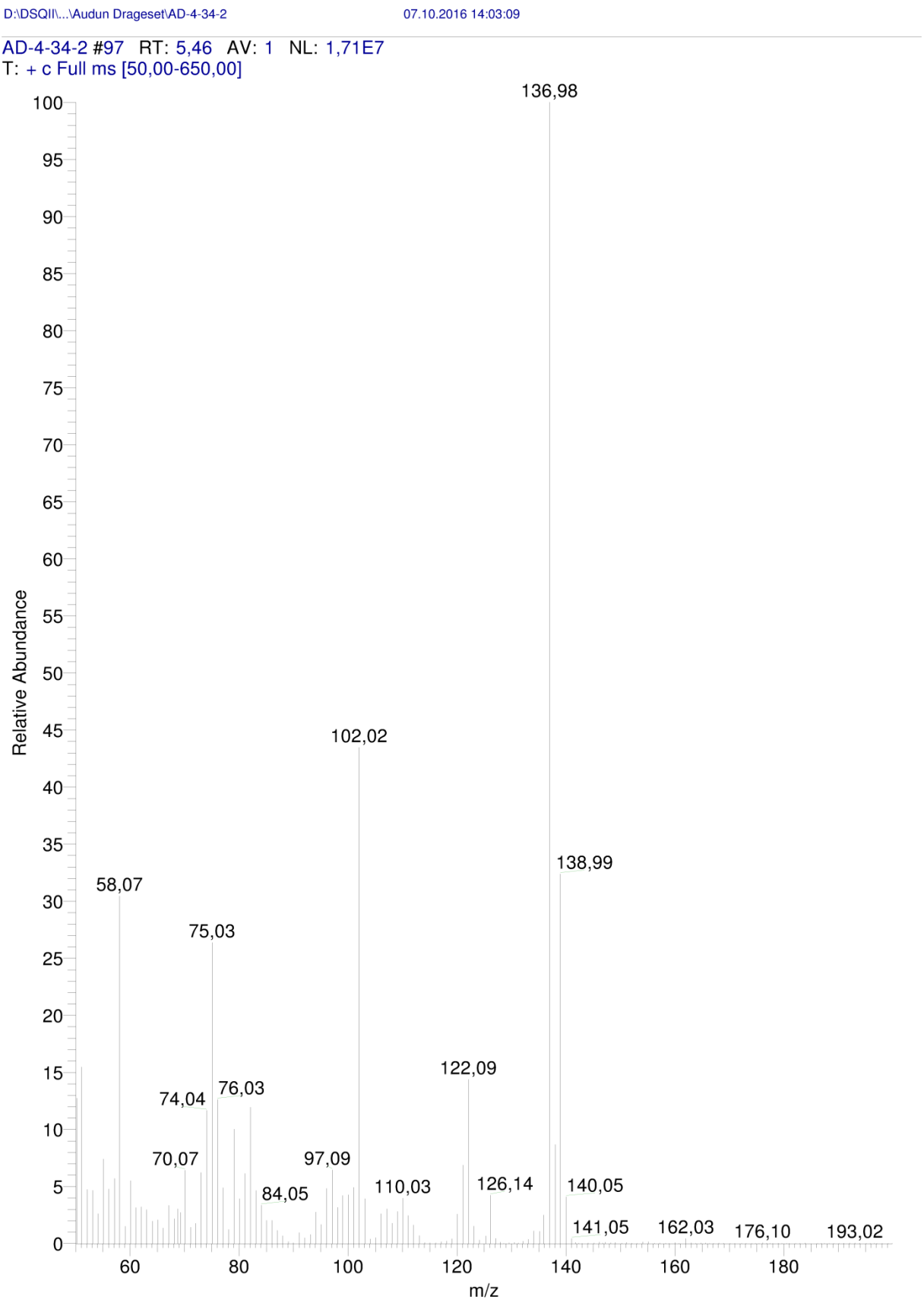
## 4-chlorobenzonitrile (3h): $^{1}$H-NMR in $CDCl_3$



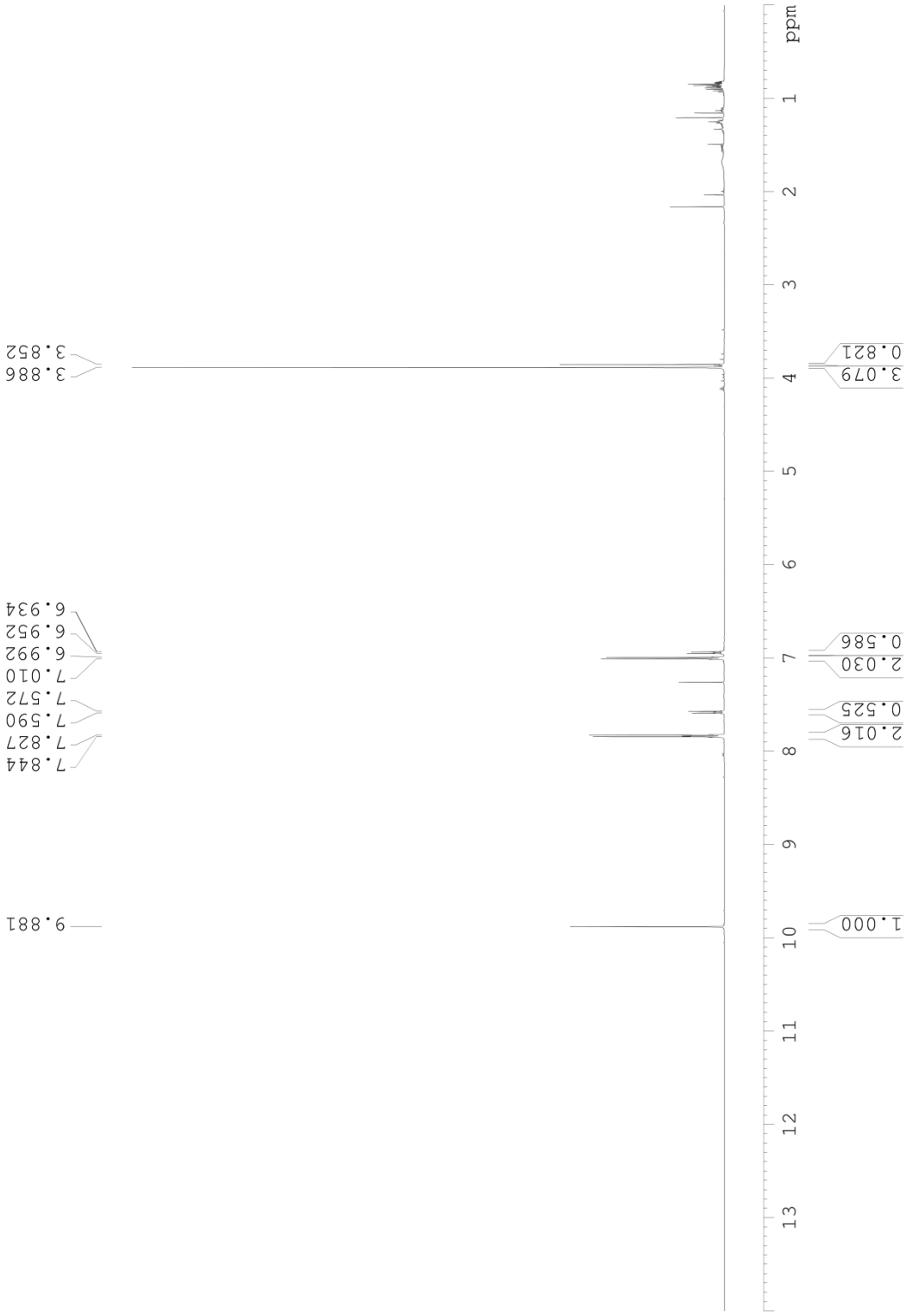
## 4-chlorobenzonitrile (3h): $^{13}$C-NMR in $CDCl_3$



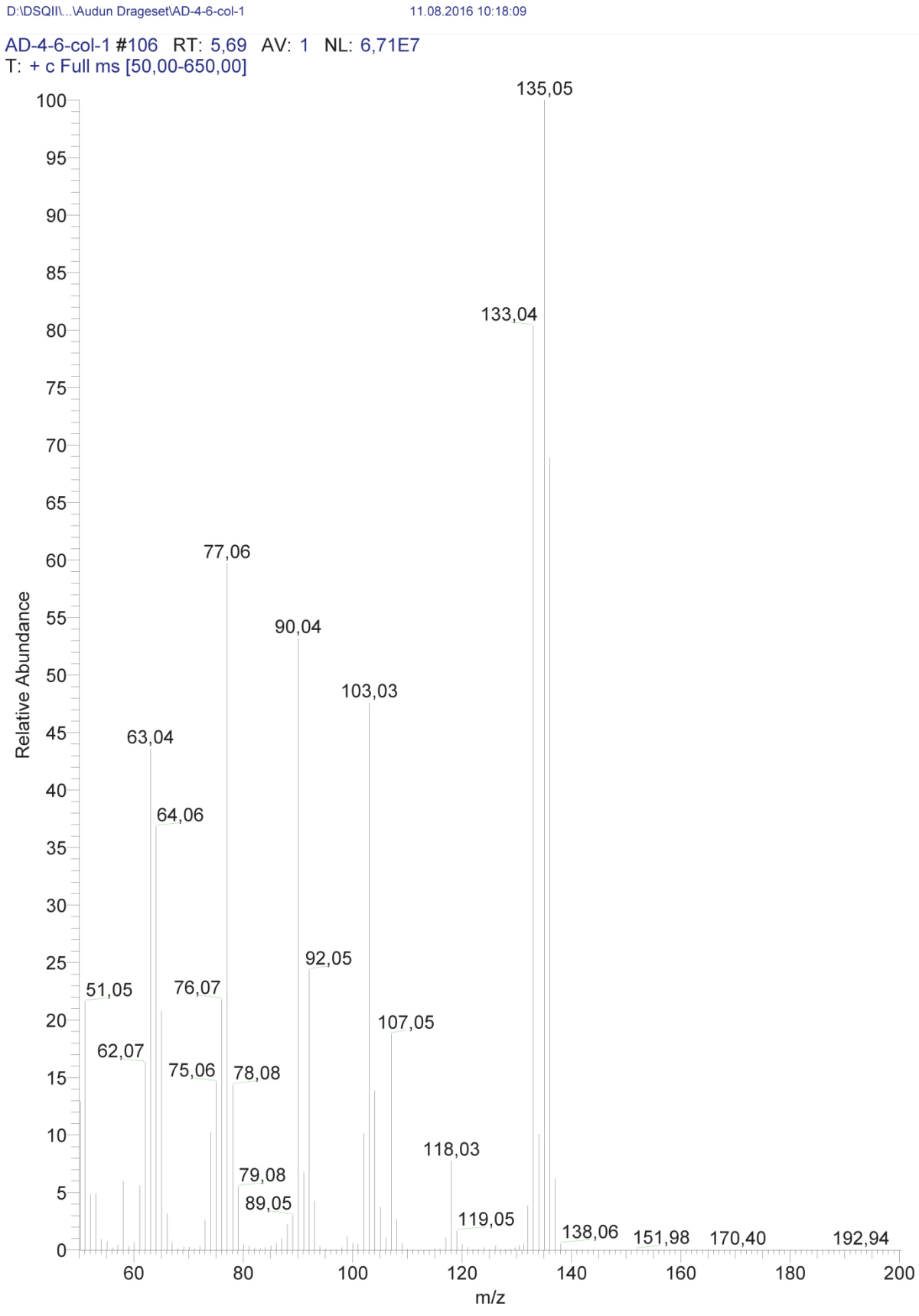
## 4-chlorobenzonitrile (3h): GC-MS



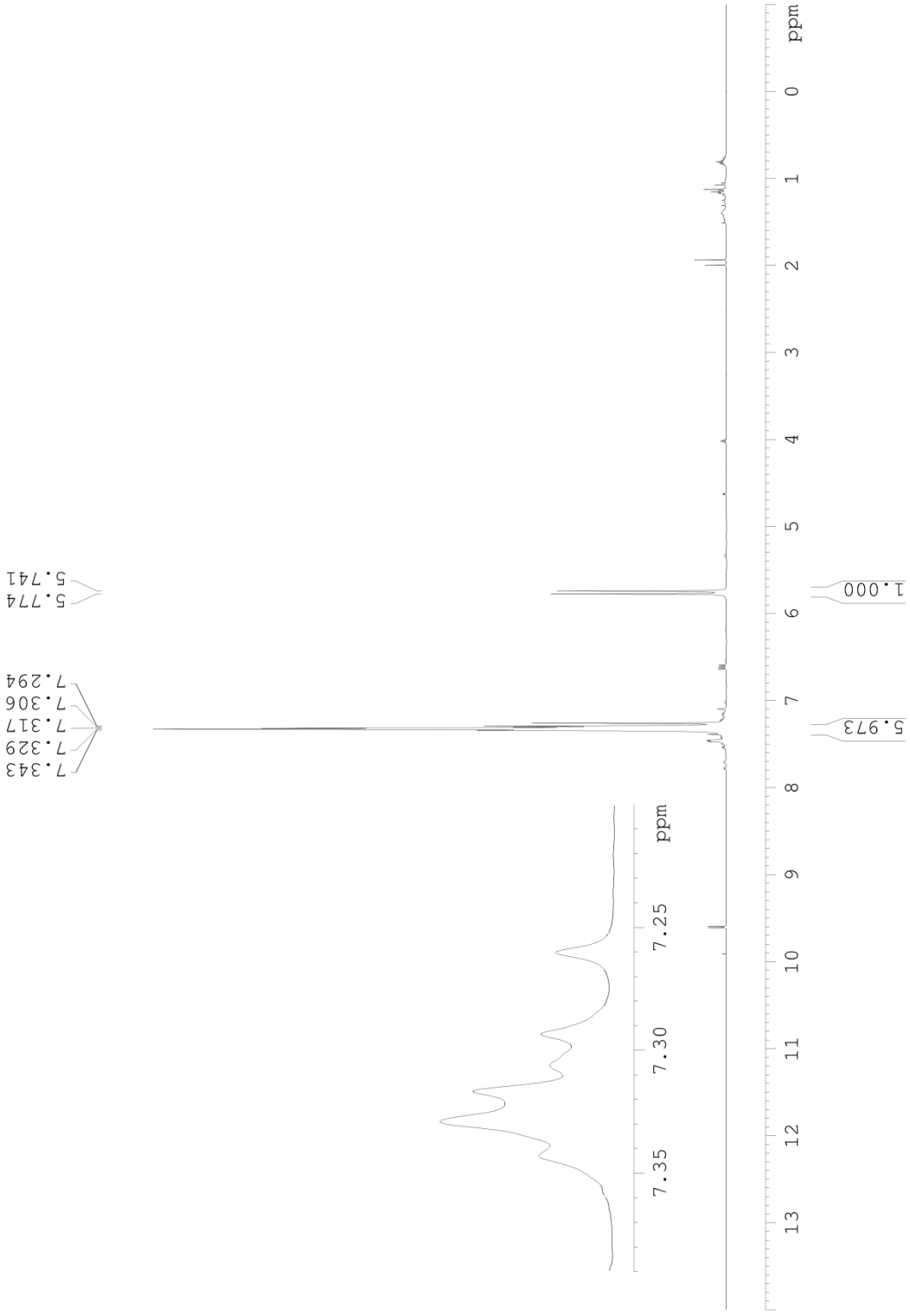
## 4-methoxybenzylalcohol (2i) + 4-methoxybenzonitrile (3i) mixture: $^{1}$H-NMR in $CDCl_3$



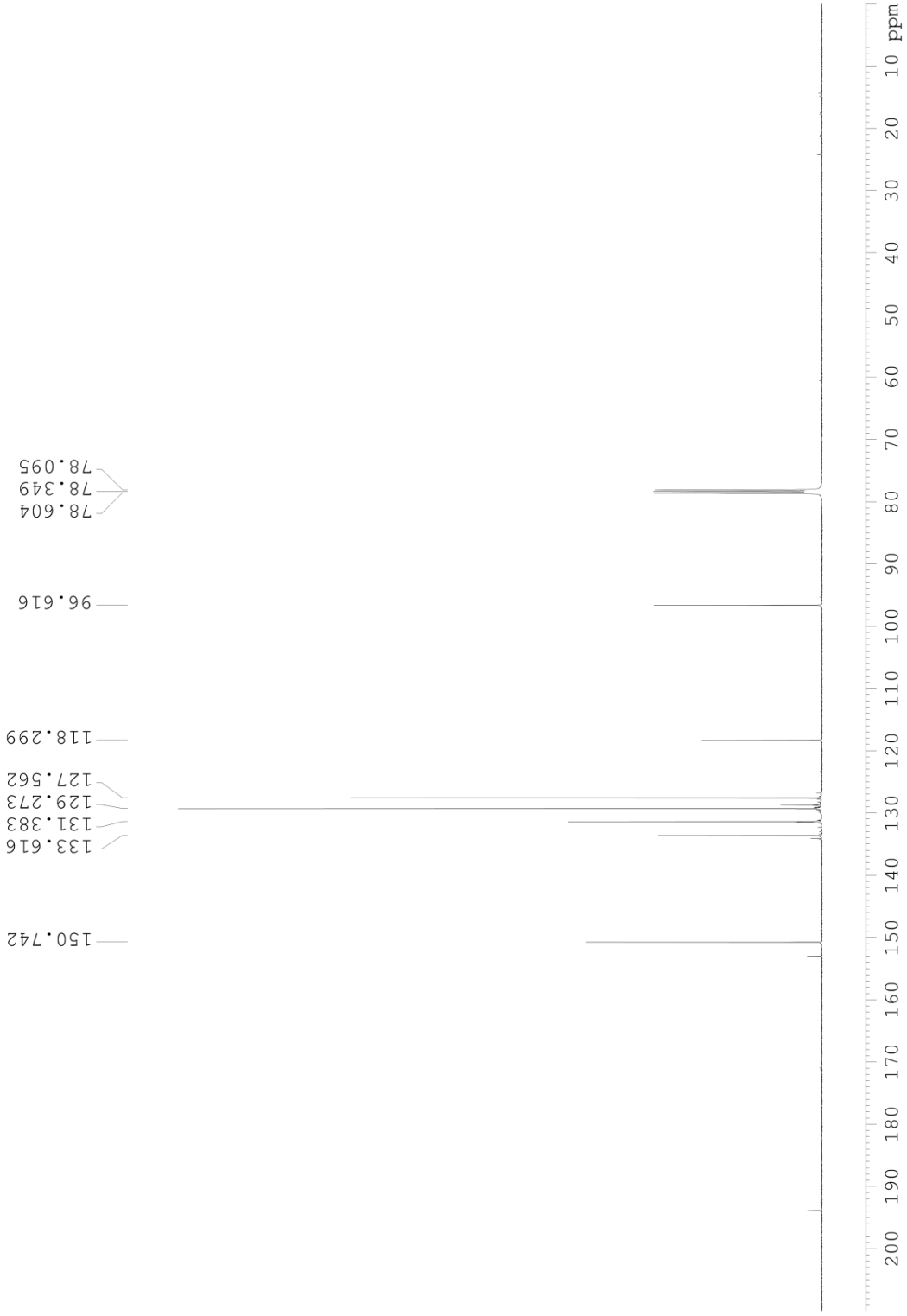
## 4-methoxybenzylalcohol (2i) + 4-methoxybenzonitrile (3i) mixture: GC-MS



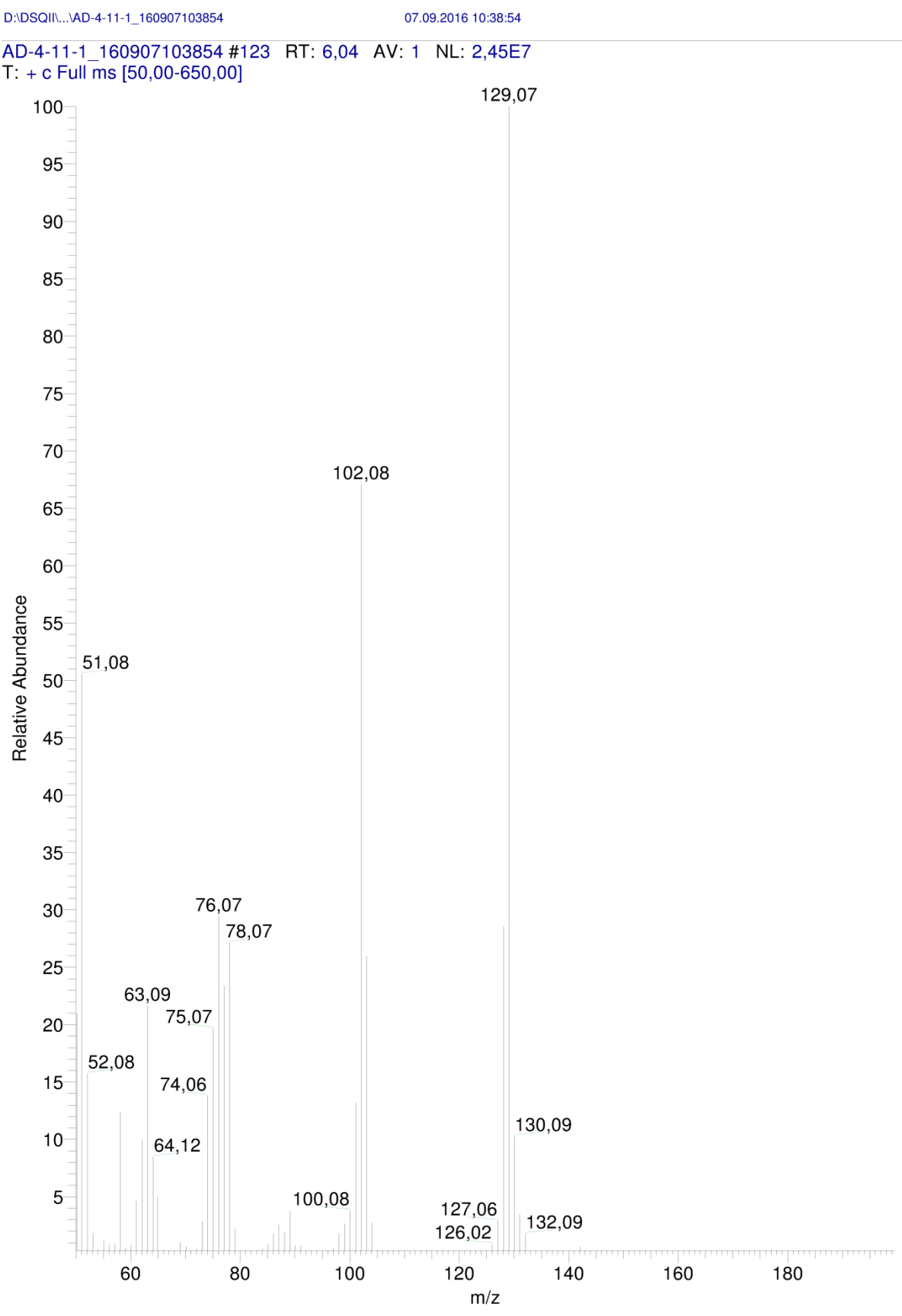
## Cinnamonitrile (3j): $^{1}$H-NMR in $CDCl_3$



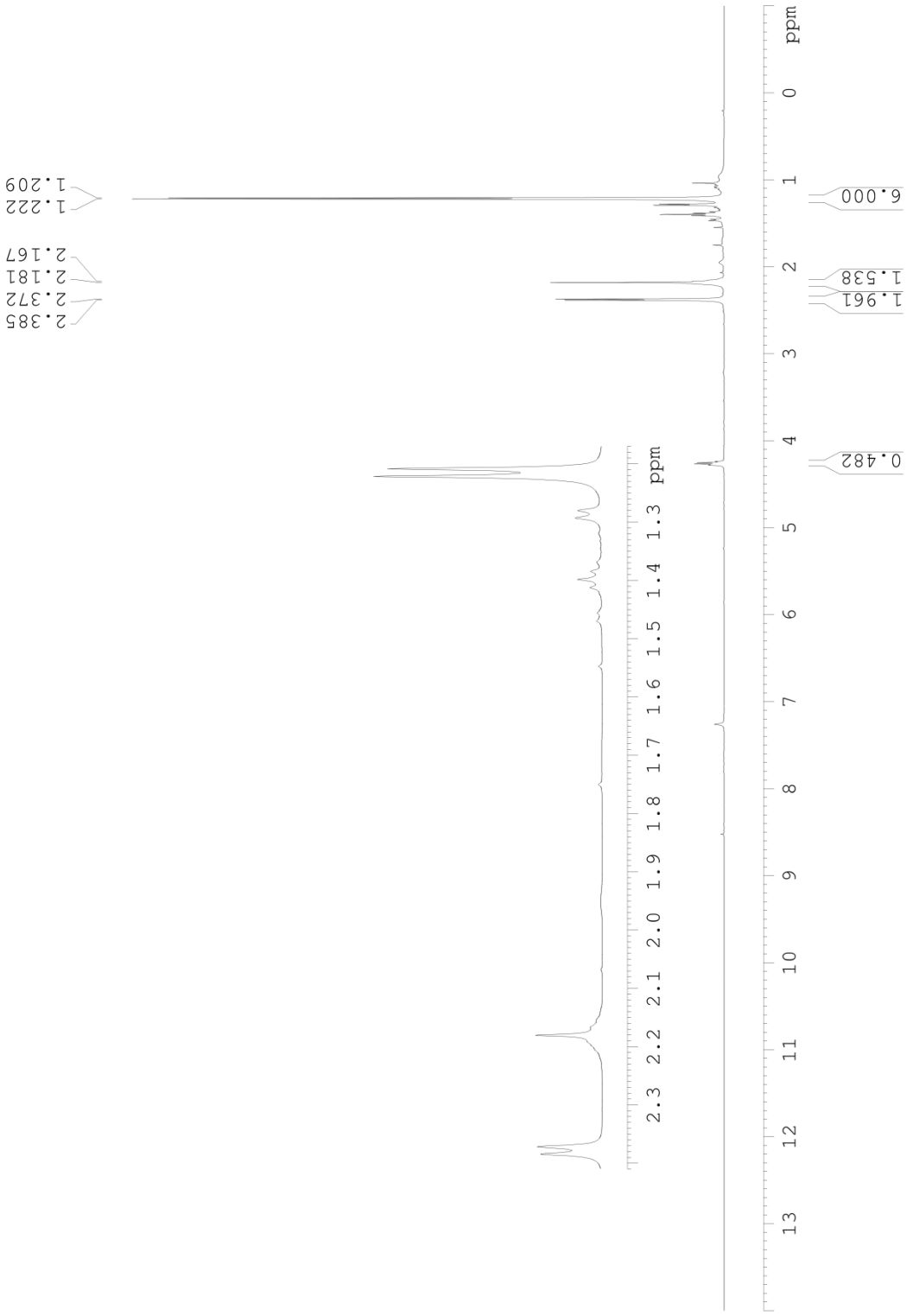
## Cinnamonitrile (3j): $^{13}$C-NMR in $CDCl_3$



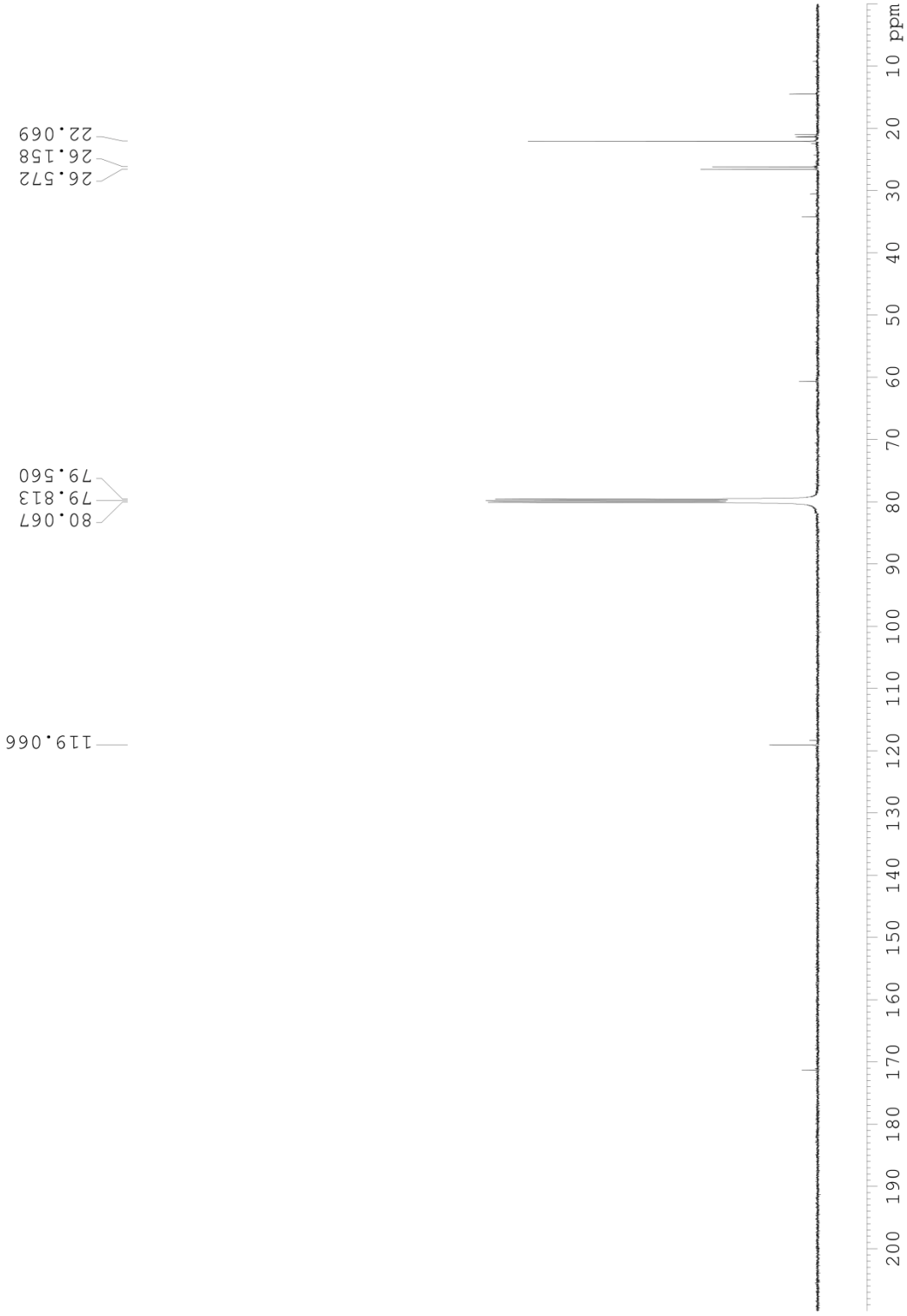
## Cinnamonitrile (3j): GC-MS



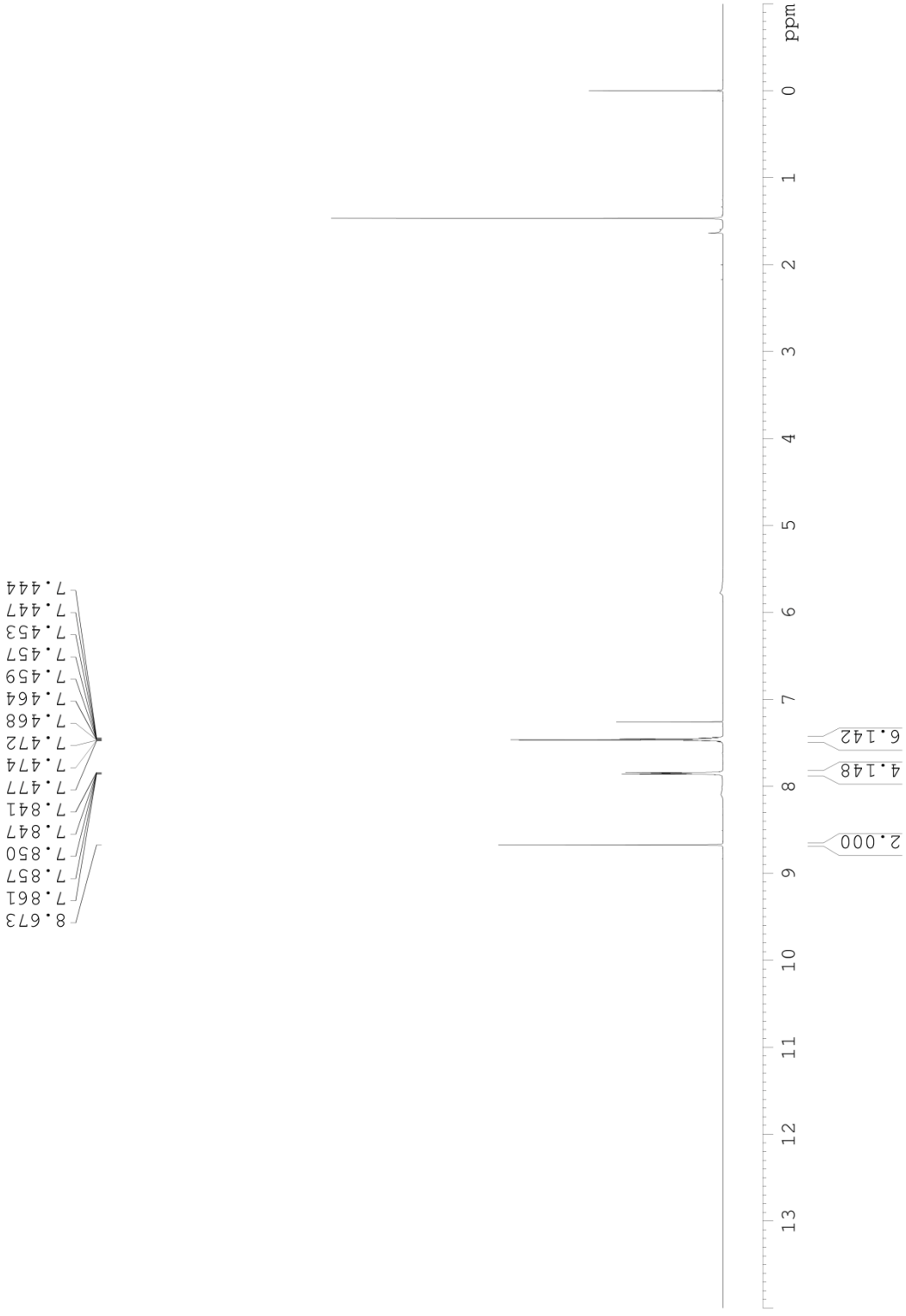
## 3-methylbutanenitrile (3k): $^{1}$H-NMR in $CDCl_3$



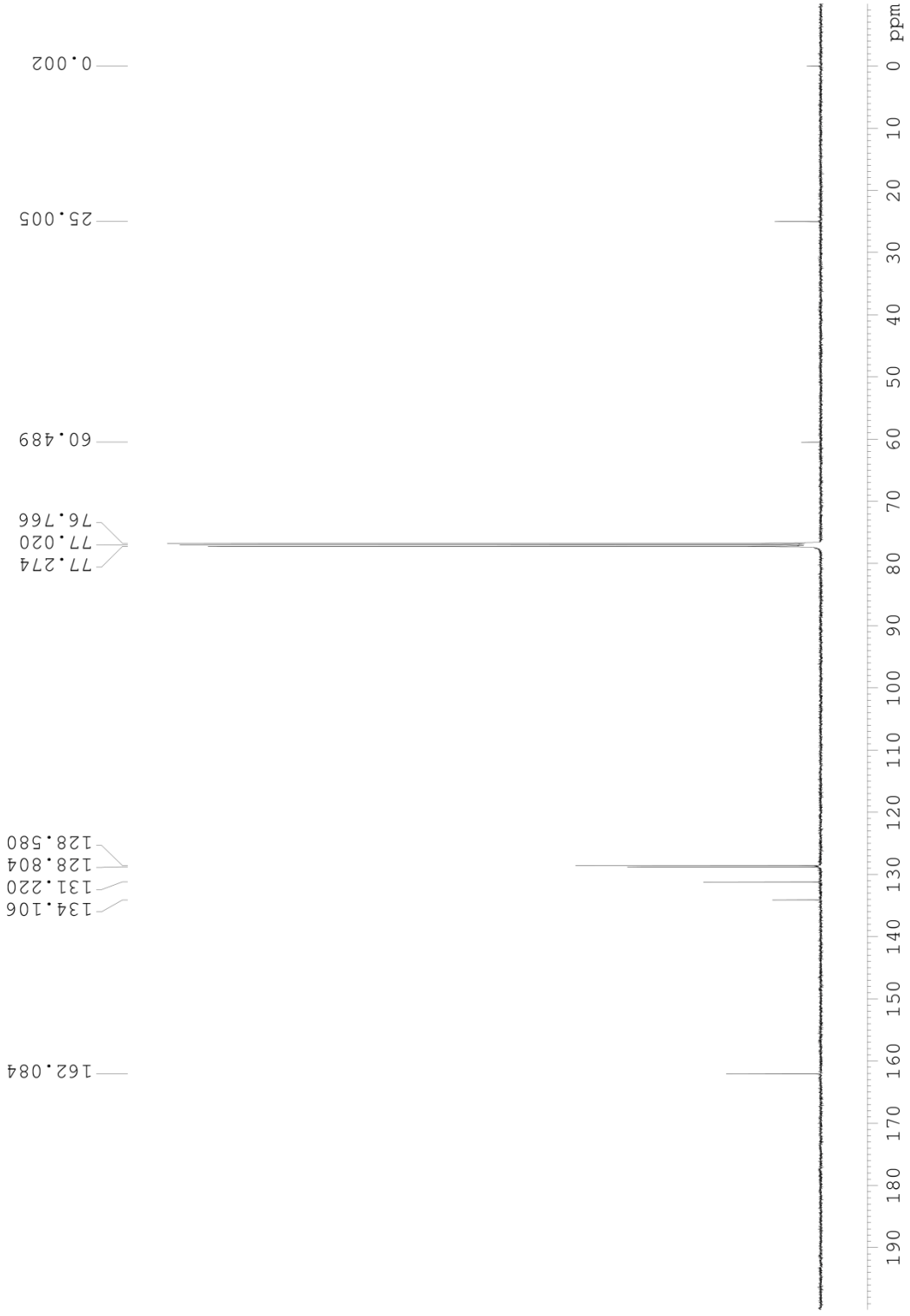
## 3-methylbutanenitrile (3k): $^{13}$C-NMR in $CDCl_3$



## 1,2-di((E)-benzylidene)hydrazine (4): $^{1}$H-NMR in $CDCl_3$



## 1,2-di((E)-benzylidene)hydrazine (4): $^{13}$C-NMR in $CDCl_3$




## 1,2-di((E)-benzylidene)hydrazine (4): X-ray crystallography

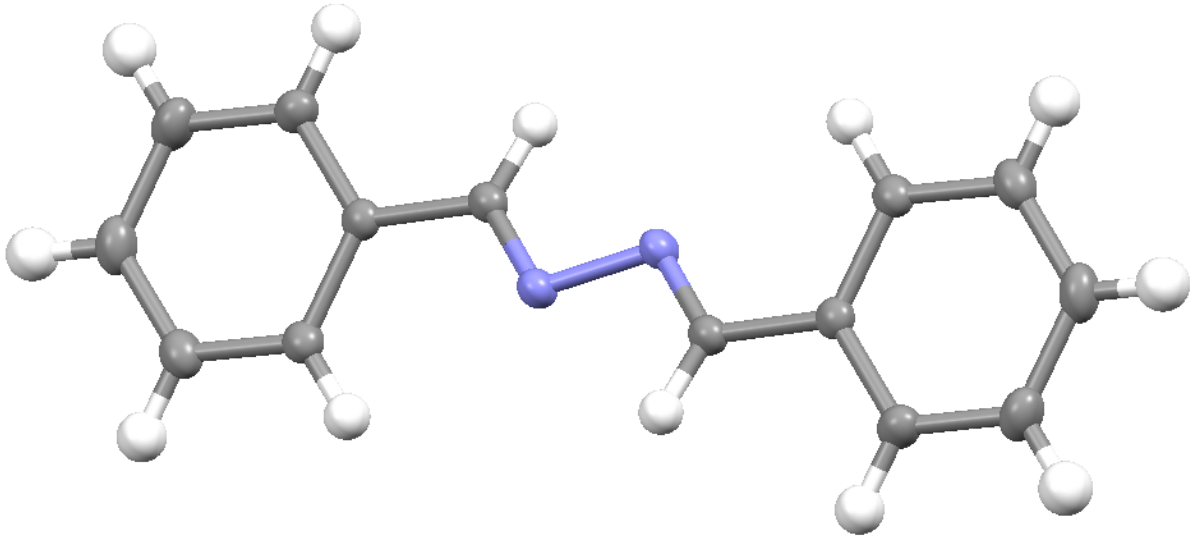


**Figure 1: X-ray structure of 1,2-di((E)-benzylidene)hydrazine (4).**

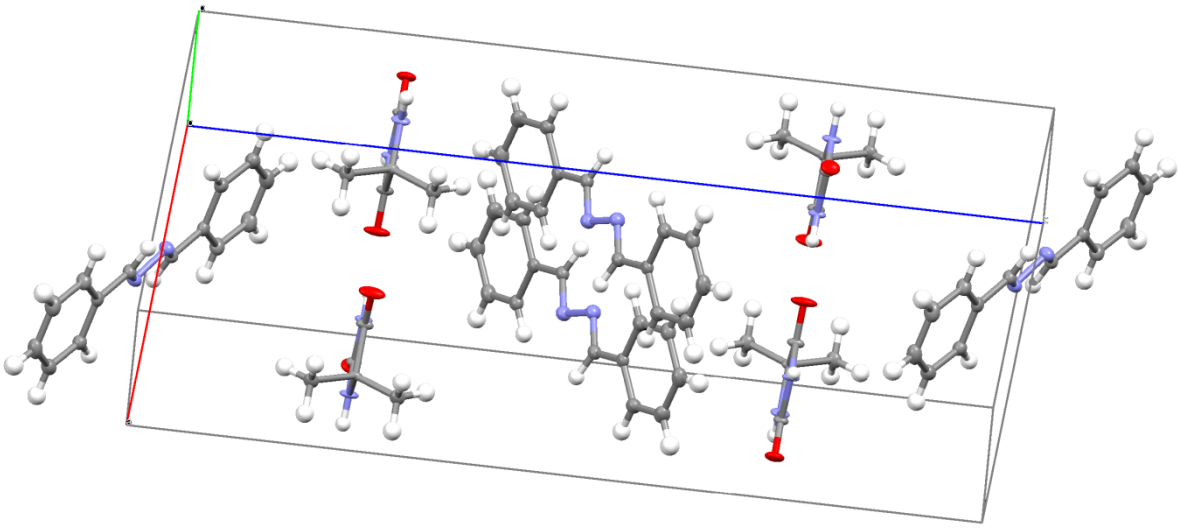


**Figure 2: 1,2-di((E)-benzylidene)hydrazine (4) cocrystallized with 5,5-dimethylhydantoin.**

## Table 1. Crystal data and structure refinement for ADUcry2.

| | | |
|---|---|---|
| Identification code | aducry2_0m_a | |
| Empirical formula | C19 H20 N4 O2 | |
| Formula weight | 336.39 | |
| Temperature | 103(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 21/c | |
| Unit cell dimensions | a = 9.7688(6) Å | α= 90°. |
| | b = 7.3520(4) Å | β= 94.2330(10)°. |
| | c = 24.5762(14) Å | γ = 90°. |
| Volume | 1760.25(18) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.269 $Mg/m^3$ | |
| Absorption coefficient | 0.085 $mm^{-1}$ | |
| F(000) | 712 | |
| Crystal size | 0.581 x 0.503 x 0.140 $mm^3$ | |
| Crystal colour/habit | Colourless/Flat prism | |
| Theta range for data collection | 1.662 to 32.046°. | |
| Index ranges | -14<=h<=14, -10<=k<=10, -36<=l<=36 | |
| Reflections collected | 32293 | |
| Independent reflections | 6112 [R(int) = 0.0497] | |
| Completeness to theta = 25.242° | 100.0 % | |
| Absorption correction | Numerical from face indexing (Gaussian quadrature) | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 6112 / 0 / 228 | |
| Goodness-of-fit on $F^2$ | 1.123 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0538, wR2 = 0.1576 | |
| R indices (all data) | R1 = 0.0633, wR2 = 0.1654 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.590 and -0.247 $e.Å^{-3}$ | |

## Table 2. Bond lengths [Å] and angles [°] for ADUcry2.

| | |
|---|---|
| O(1)-C(2) | 1.2278(11) |
| O(2)-C(4) | 1.2240(11) |
| N(1)-C(2) | 1.3429(12) |
| N(1)-C(5) | 1.4612(12) |
| N(1)-H(1) | 0.8800 |
| N(3)-C(4) | 1.3521(11) |
| N(3)-C(2) | 1.3993(11) |
| N(3)-H(3) | 0.8800 |
| N(4)-C(8) | 1.2820(14) |
| N(4)-N(5) | 1.4110(14) |
| N(5)-C(15) | 1.2816(14) |
| C(4)-C(5) | 1.5203(12) |
| C(5)-C(6) | 1.5262(14) |
| C(5)-C(7) | 1.5285(14) |
| C(6)-H(6A) | 0.9800 |
| C(6)-H(6B) | 0.9800 |
| C(6)-H(6C) | 0.9800 |
| C(7)-H(7A) | 0.9800 |
| C(7)-H(7B) | 0.9800 |
| C(7)-H(7C) | 0.9800 |
| C(8)-C(9) | 1.4625(15) |
| C(8)-H(8) | 0.9500 |

| | |
|---|---|
| C(9)-C(14) | 1.3983(15) |
| C(9)-C(10) | 1.4017(15) |
| C(10)-C(11) | 1.3896(16) |
| C(10)-H(10) | 0.9500 |
| C(11)-C(12) | 1.3914(18) |
| C(11)-H(11) | 0.9500 |
| C(12)-C(13) | 1.3879(18) |
| C(12)-H(12) | 0.9500 |
| C(13)-C(14) | 1.3928(17) |
| C(13)-H(13) | 0.9500 |
| C(14)-H(14) | 0.9500 |
| C(15)-C(16) | 1.4635(15) |
| C(15)-H(15) | 0.9500 |
| C(16)-C(17) | 1.3985(15) |
| C(16)-C(21) | 1.3999(15) |
| C(17)-C(18) | 1.3911(17) |
| C(17)-H(17) | 0.9500 |
| C(18)-C(19) | 1.3890(19) |
| C(18)-H(18) | 0.9500 |
| C(19)-C(20) | 1.3915(18) |
| C(19)-H(19) | 0.9500 |
| C(20)-C(21) | 1.3883(16) |
| C(20)-H(20) | 0.9500 |
| C(21)-H(21) | 0.9500 |

| | |
|---|---|
| C(2)-N(1)-C(5) | 113.01(7) |
| C(2)-N(1)-H(1) | 123.5 |
| C(5)-N(1)-H(1) | 123.5 |
| C(4)-N(3)-C(2) | 111.69(7) |
| C(4)-N(3)-H(3) | 124.2 |
| C(2)-N(3)-H(3) | 124.2 |
| C(8)-N(4)-N(5) | 111.39(9) |
| C(15)-N(5)-N(4) | 111.33(9) |
| O(1)-C(2)-N(1) | 129.59(8) |
| O(1)-C(2)-N(3) | 123.41(8) |
| N(1)-C(2)-N(3) | 107.01(7) |
| O(2)-C(4)-N(3) | 124.66(8) |
| O(2)-C(4)-C(5) | 127.51(8) |
| N(3)-C(4)-C(5) | 107.82(7) |
| N(1)-C(5)-C(4) | 100.47(7) |
| N(1)-C(5)-C(6) | 111.75(8) |
| C(4)-C(5)-C(6) | 110.46(8) |
| N(1)-C(5)-C(7) | 111.70(8) |
| C(4)-C(5)-C(7) | 110.31(8) |
| C(6)-C(5)-C(7) | 111.64(8) |
| C(5)-C(6)-H(6A) | 109.5 |
| C(5)-C(6)-H(6B) | 109.5 |
| H(6A)-C(6)-H(6B) | 109.5 |
| C(5)-C(6)-H(6C) | 109.5 |
| H(6A)-C(6)-H(6C) | 109.5 |
| H(6B)-C(6)-H(6C) | 109.5 |
| C(5)-C(7)-H(7A) | 109.5 |
| C(5)-C(7)-H(7B) | 109.5 |
| H(7A)-C(7)-H(7B) | 109.5 |
| C(5)-C(7)-H(7C) | 109.5 |
| H(7A)-C(7)-H(7C) | 109.5 |
| H(7B)-C(7)-H(7C) | 109.5 |
| N(4)-C(8)-C(9) | 121.89(9) |
| N(4)-C(8)-H(8) | 119.1 |
| C(9)-C(8)-H(8) | 119.1 |
| C(14)-C(9)-C(10) | 119.53(10) |
| C(14)-C(9)-C(8) | 118.93(9) |
| C(10)-C(9)-C(8) | 121.54(10) |
| C(11)-C(10)-C(9) | 119.84(10) |
| C(11)-C(10)-H(10) | 120.1 |

| | |
|---|---|
| C(9)-C(10)-H(10) | 120.1 |
| C(10)-C(11)-C(12) | 120.36(11) |
| C(10)-C(11)-H(11) | 119.8 |
| C(12)-C(11)-H(11) | 119.8 |
| C(13)-C(12)-C(11) | 120.06(11) |
| C(13)-C(12)-H(12) | 120.0 |
| C(11)-C(12)-H(12) | 120.0 |
| C(12)-C(13)-C(14) | 120.05(11) |
| C(12)-C(13)-H(13) | 120.0 |
| C(14)-C(13)-H(13) | 120.0 |
| C(13)-C(14)-C(9) | 120.15(11) |
| C(13)-C(14)-H(14) | 119.9 |
| C(9)-C(14)-H(14) | 119.9 |
| N(5)-C(15)-C(16) | 121.94(9) |
| N(5)-C(15)-H(15) | 119.0 |
| C(16)-C(15)-H(15) | 119.0 |
| C(17)-C(16)-C(21) | 119.57(10) |
| C(17)-C(16)-C(15) | 118.85(9) |
| C(21)-C(16)-C(15) | 121.58(10) |
| C(18)-C(17)-C(16) | 120.11(11) |
| C(18)-C(17)-H(17) | 119.9 |
| C(16)-C(17)-H(17) | 119.9 |
| C(19)-C(18)-C(17) | 120.09(11) |
| C(19)-C(18)-H(18) | 120.0 |
| C(17)-C(18)-H(18) | 120.0 |
| C(18)-C(19)-C(20) | 119.99(11) |
| C(18)-C(19)-H(19) | 120.0 |
| C(20)-C(19)-H(19) | 120.0 |
| C(21)-C(20)-C(19) | 120.35(11) |
| C(21)-C(20)-H(20) | 119.8 |
| C(19)-C(20)-H(20) | 119.8 |
| C(20)-C(21)-C(16) | 119.89(10) |
| C(20)-C(21)-H(21) | 120.1 |
| C(16)-C(21)-H(21) | 120.1 |

Symmetry transformations used to generate equivalent atoms:

## Table 3. Torsion angles [°] for ADUcry2.

| | |
|---|---|
| C(8)-N(4)-N(5)-C(15) | 179.92(9) |
| C(5)-N(1)-C(2)-O(1) | -179.47(10) |
| C(5)-N(1)-C(2)-N(3) | 0.33(12) |
| C(4)-N(3)-C(2)-O(1) | 179.24(10) |
| C(4)-N(3)-C(2)-N(1) | -0.57(12) |
| C(2)-N(3)-C(4)-O(2) | -179.10(11) |
| C(2)-N(3)-C(4)-C(5) | 0.57(12) |
| C(2)-N(1)-C(5)-C(4) | 0.00(11) |
| C(2)-N(1)-C(5)-C(6) | 117.16(9) |
| C(2)-N(1)-C(5)-C(7) | -116.97(9) |
| O(2)-C(4)-C(5)-N(1) | 179.31(12) |
| N(3)-C(4)-C(5)-N(1) | -0.34(10) |
| O(2)-C(4)-C(5)-C(6) | 61.20(14) |
| N(3)-C(4)-C(5)-C(6) | -118.45(9) |
| O(2)-C(4)-C(5)-C(7) | -62.70(14) |
| N(3)-C(4)-C(5)-C(7) | 117.65(9) |
| N(5)-N(4)-C(8)-C(9) | -179.14(9) |
| N(4)-C(8)-C(9)-C(14) | 161.62(10) |
| N(4)-C(8)-C(9)-C(10) | -17.61(16) |
| C(14)-C(9)-C(10)-C(11) | -0.80(16) |
| C(8)-C(9)-C(10)-C(11) | 178.43(10) |
| C(9)-C(10)-C(11)-C(12) | -0.05(17) |
| C(10)-C(11)-C(12)-C(13) | 0.44(18) |
| C(11)-C(12)-C(13)-C(14) | 0.02(18) |
| C(12)-C(13)-C(14)-C(9) | -0.88(18) |

| | |
|---|---|
| C(10)-C(9)-C(14)-C(13) | 1.26(16) |
| C(8)-C(9)-C(14)-C(13) | -177.99(10) |
| N(4)-N(5)-C(15)-C(16) | 179.12(9) |
| N(5)-C(15)-C(16)-C(17) | -161.74(10) |
| N(5)-C(15)-C(16)-C(21) | 17.65(16) |
| C(21)-C(16)-C(17)-C(18) | -1.17(16) |
| C(15)-C(16)-C(17)-C(18) | 178.24(10) |
| C(16)-C(17)-C(18)-C(19) | 0.87(18) |
| C(17)-C(18)-C(19)-C(20) | -0.18(18) |
| C(18)-C(19)-C(20)-C(21) | -0.20(18) |
| C(19)-C(20)-C(21)-C(16) | -0.10(17) |
| C(17)-C(16)-C(21)-C(20) | 0.78(16) |
| C(15)-C(16)-C(21)-C(20) | -178.60(10) |

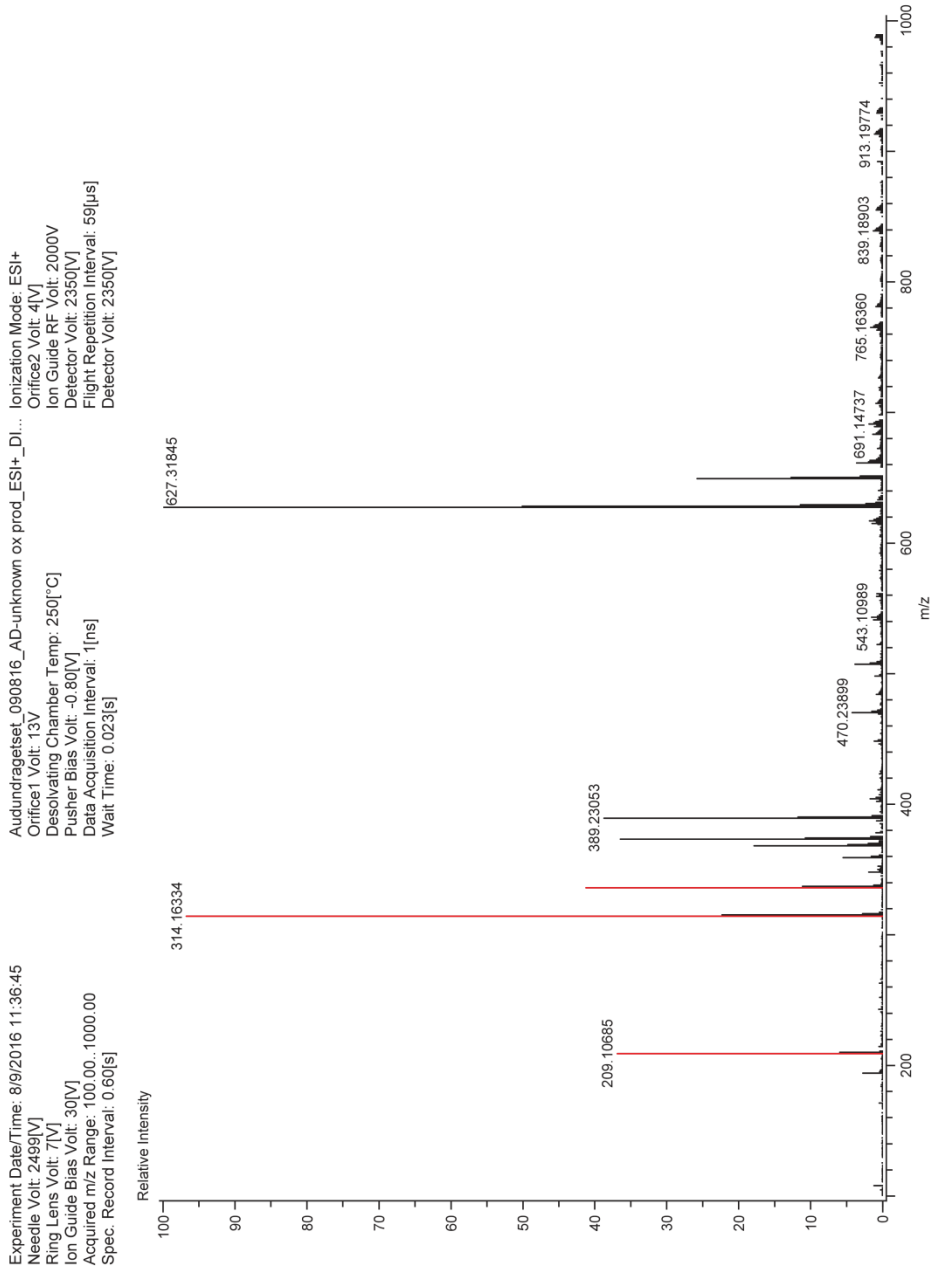
Symmetry transformations used to generate equivalent atoms:

## Table 4. Hydrogen bonds for ADUcry2 [Å and °].

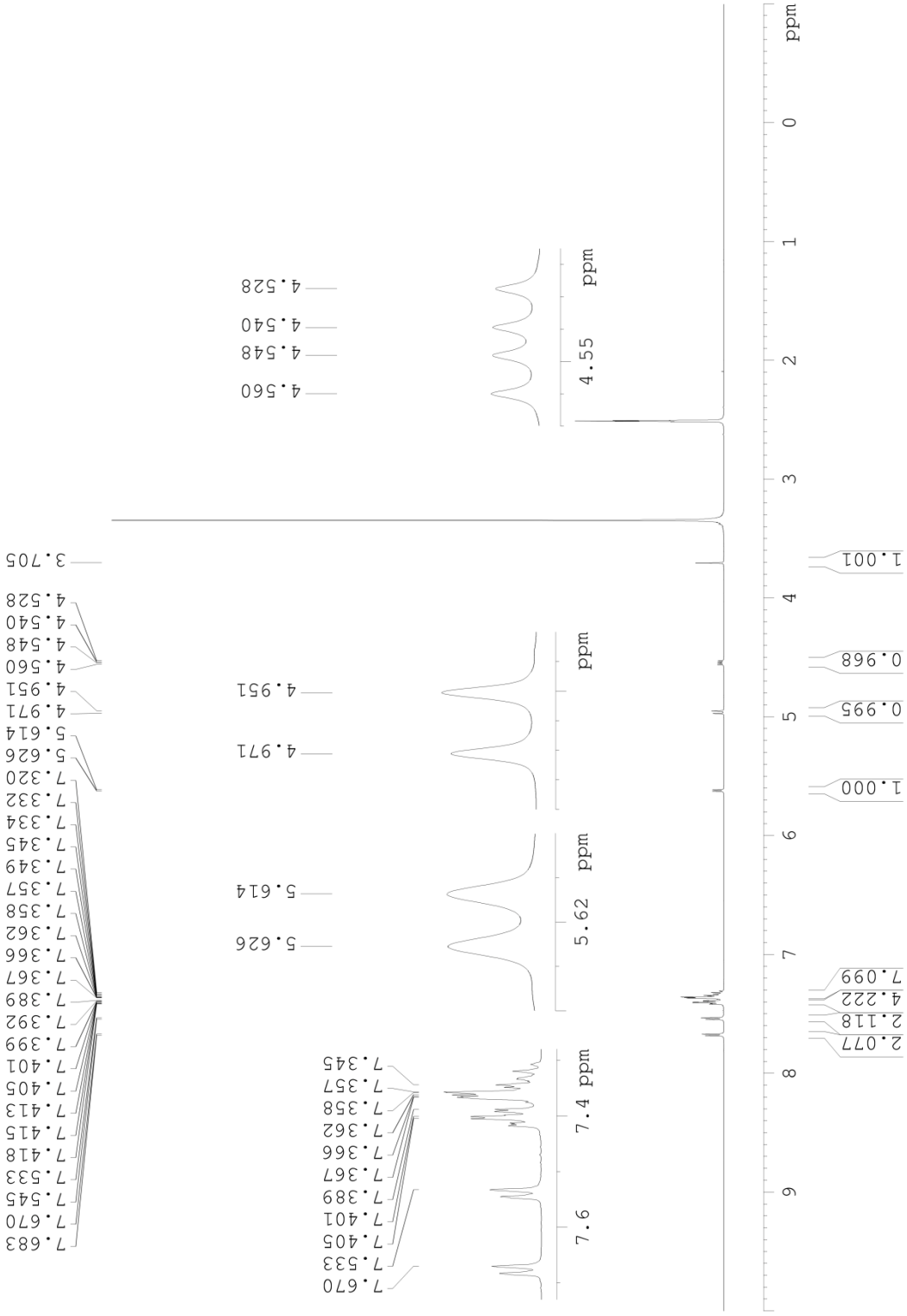
| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N(1)-H(1)...O(1)#1 | 0.88 | 1.95 | 2.7981(10) | 160.1 |
| N(3)-H(3)...O(2)#2 | 0.88 | 1.90 | 2.7719(11) | 172.1 |
| C(6)-H(6A)...O(2)#3 | 0.98 | 2.63 | 3.5119(13) | 149.7 |

Symmetry transformations used to generate equivalent atoms:
#1 -x,y-1/2,-z+1/2 #2 -x+1,y+1/2,-z+1/2 #3 -x+1,y-1/2,-z+1/2

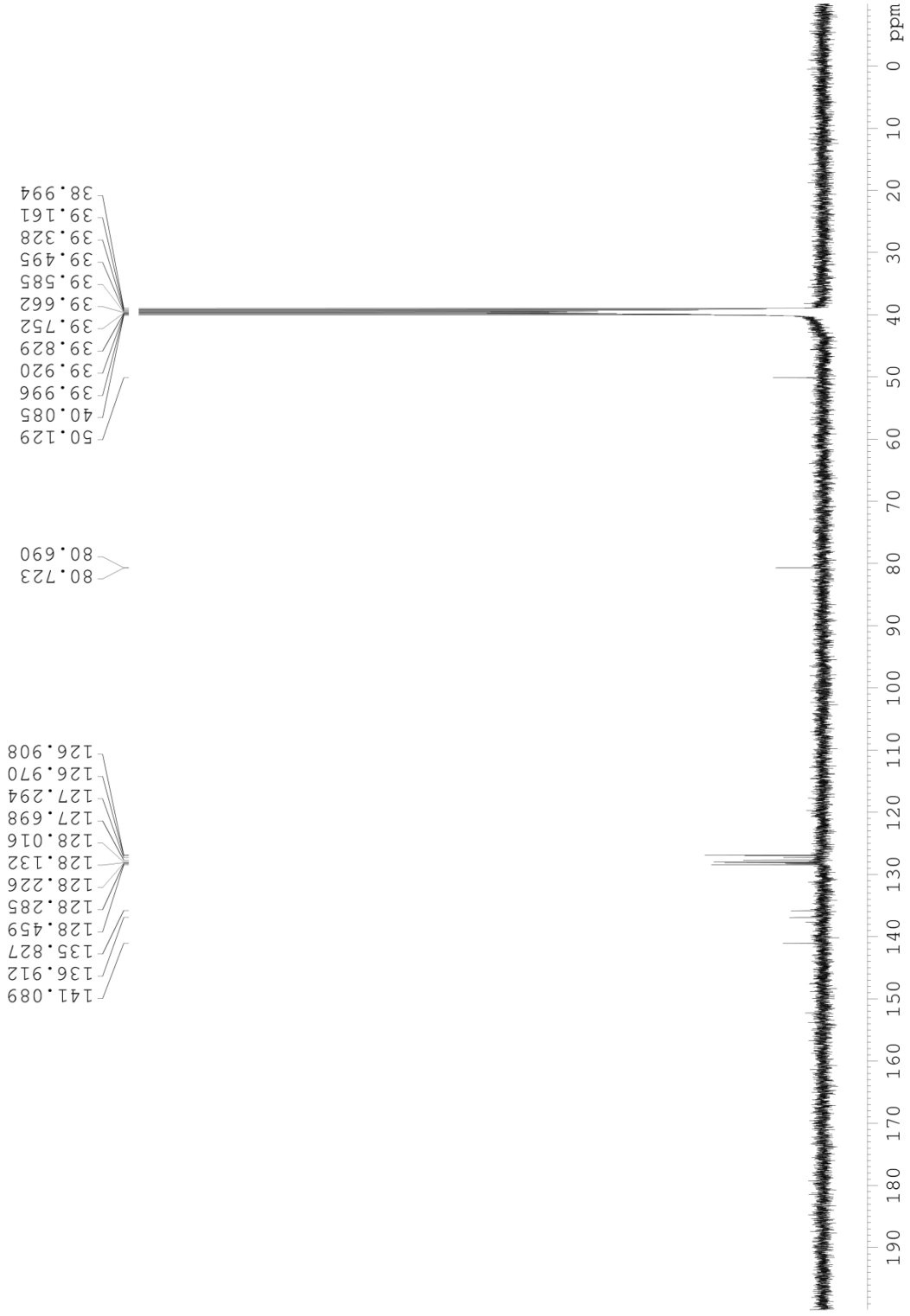
## (2R,4R)-2,4,6-triphenyl-1,3,5-triazabicyclo[3.1.0]hexane (5a): HRMS



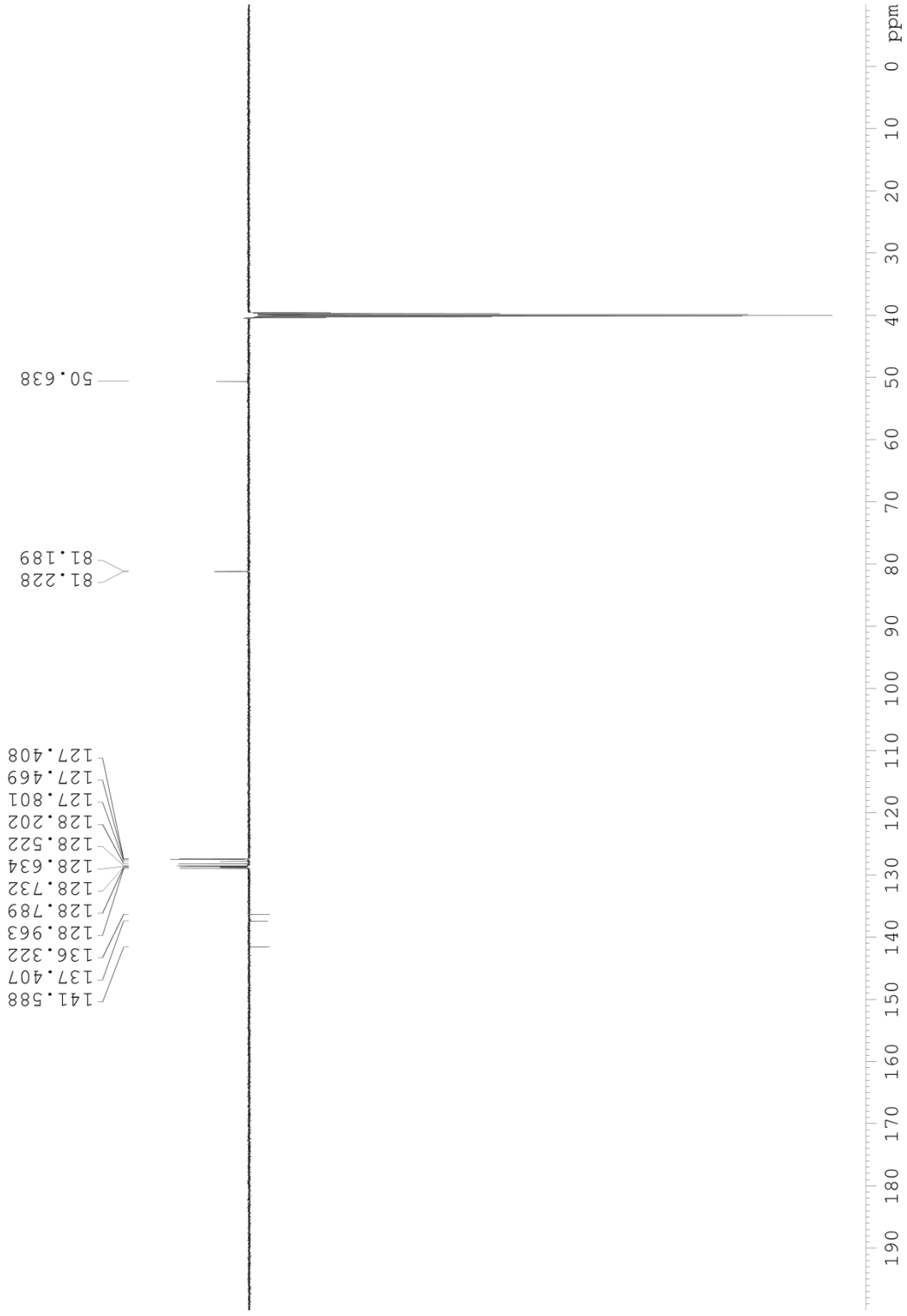
## (2R,4R)-2,4,6-triphenyl-1,3,5-triazabicyclo[3.1.0]hexane (5a): $^{1}$H-NMR in DMSO



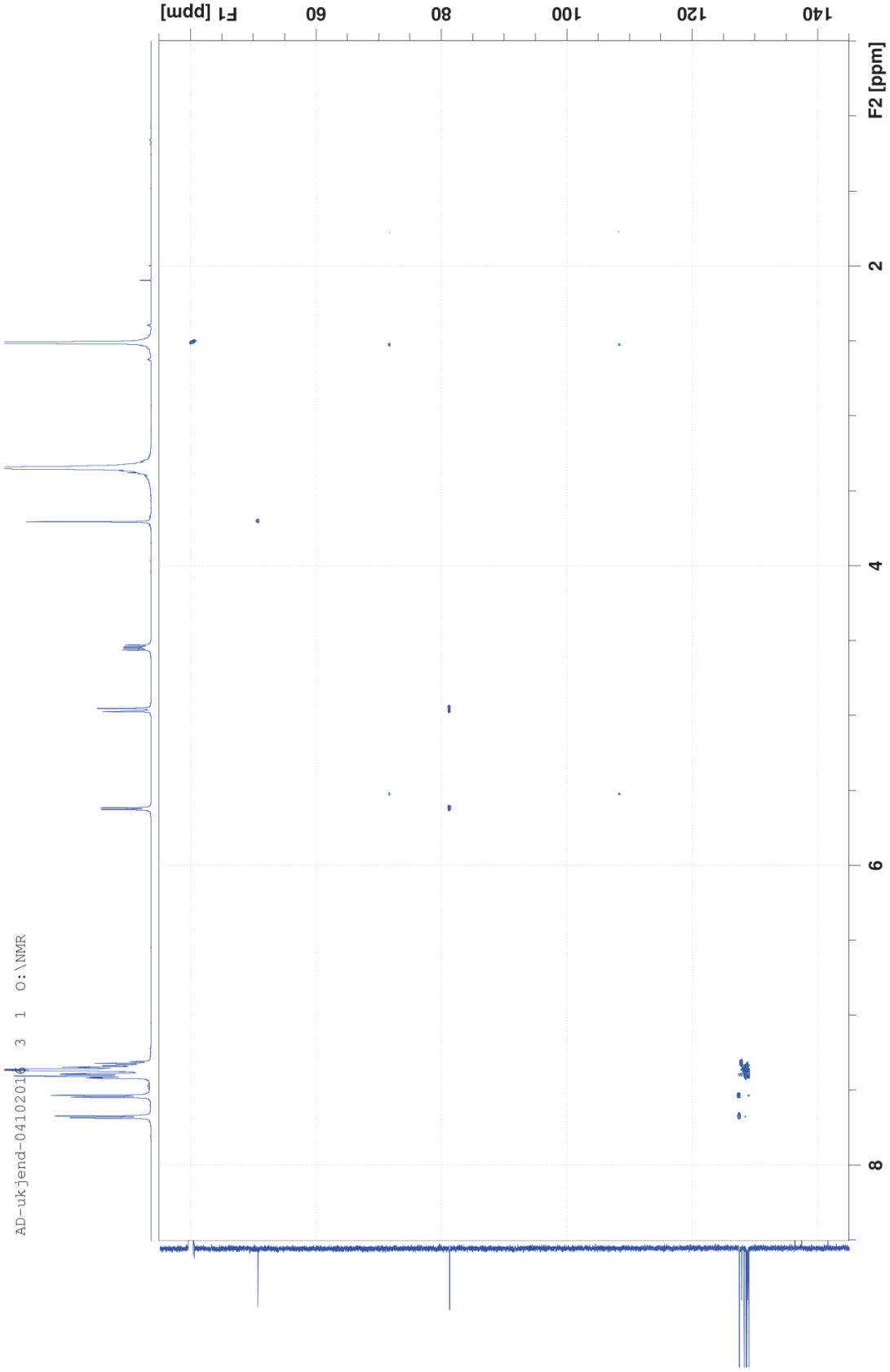
## (2R,4R)-2,4,6-triphenyl-1,3,5-triazabicyclo[3.1.0]hexane (5a): $^{13}$C-NMR in DMSO



## (2R,4R)-2,4,6-triphenyl-1,3,5-triazabicyclo[3.1.0]hexane (5a): DEPT135

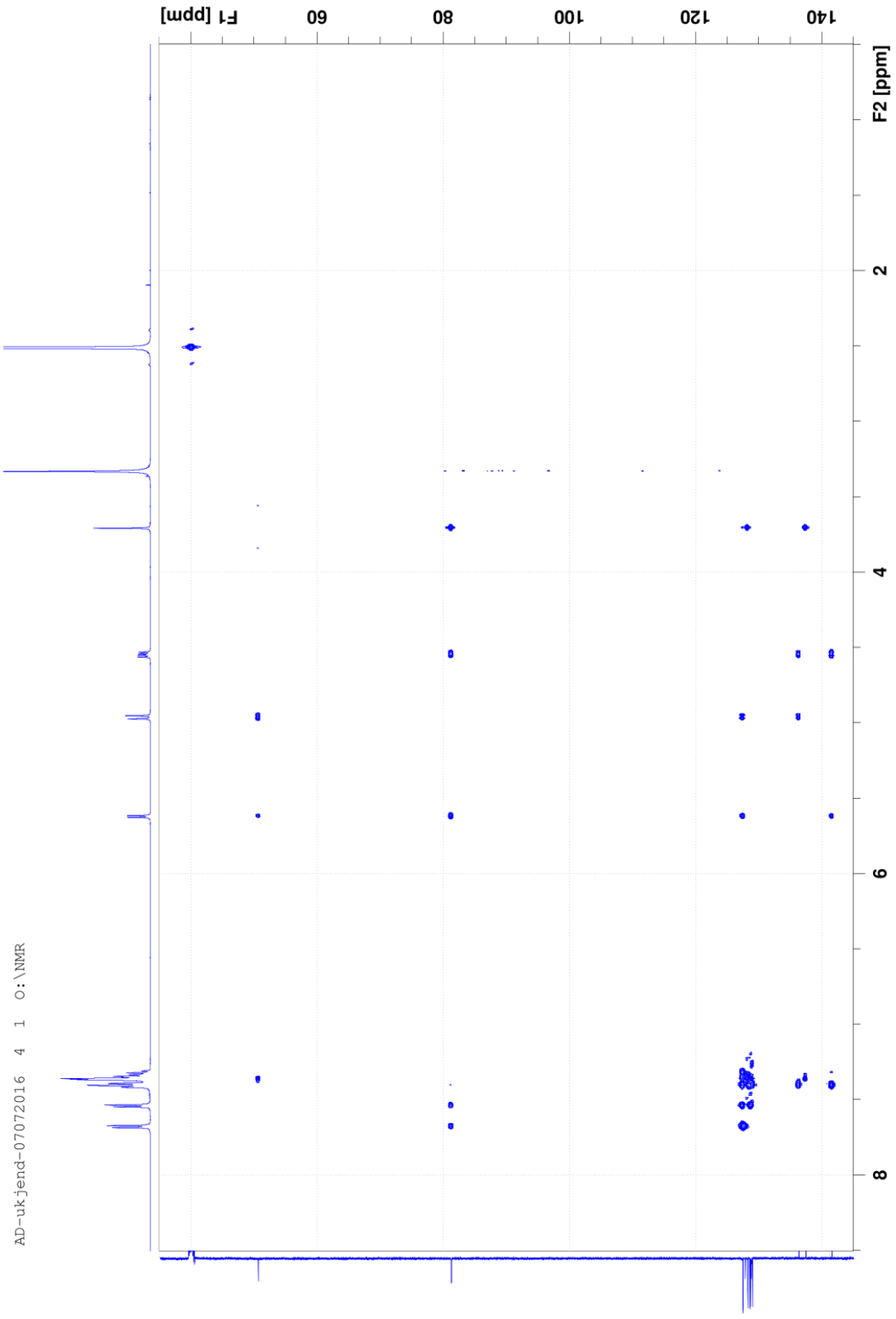


## (2R,4R)-2,4,6-triphenyl-1,3,5-triazabicyclo[3.1.0]hexane (5a): HSQC (600 MHz), DMSO.



## (2R,4R)-2,4,6-triphenyl-1,3,5-triazabicyclo[3.1.0]hexane (5a): HMBC (600 MHz), DMSO.

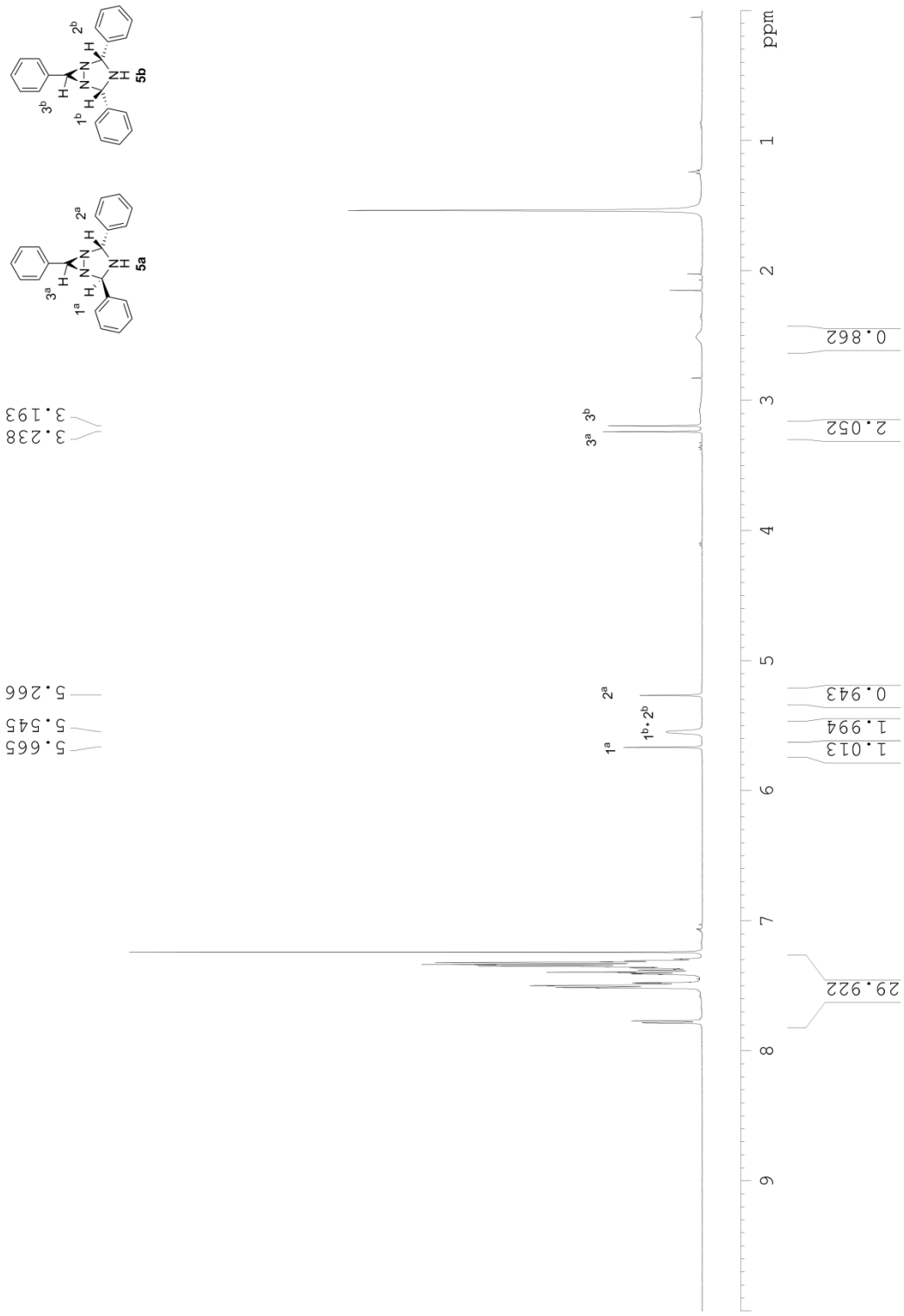
2D H-1/X correlation via heteronuclear zero and double quantum coherence phase sensitive using Echo/Antiecho gradient selection with three-fold low-pass J-filter to suppress one-bond correlations no decoupling during acquisition. Optimized for $nJ_{CH}$ = 10 Hz coupling.[1]



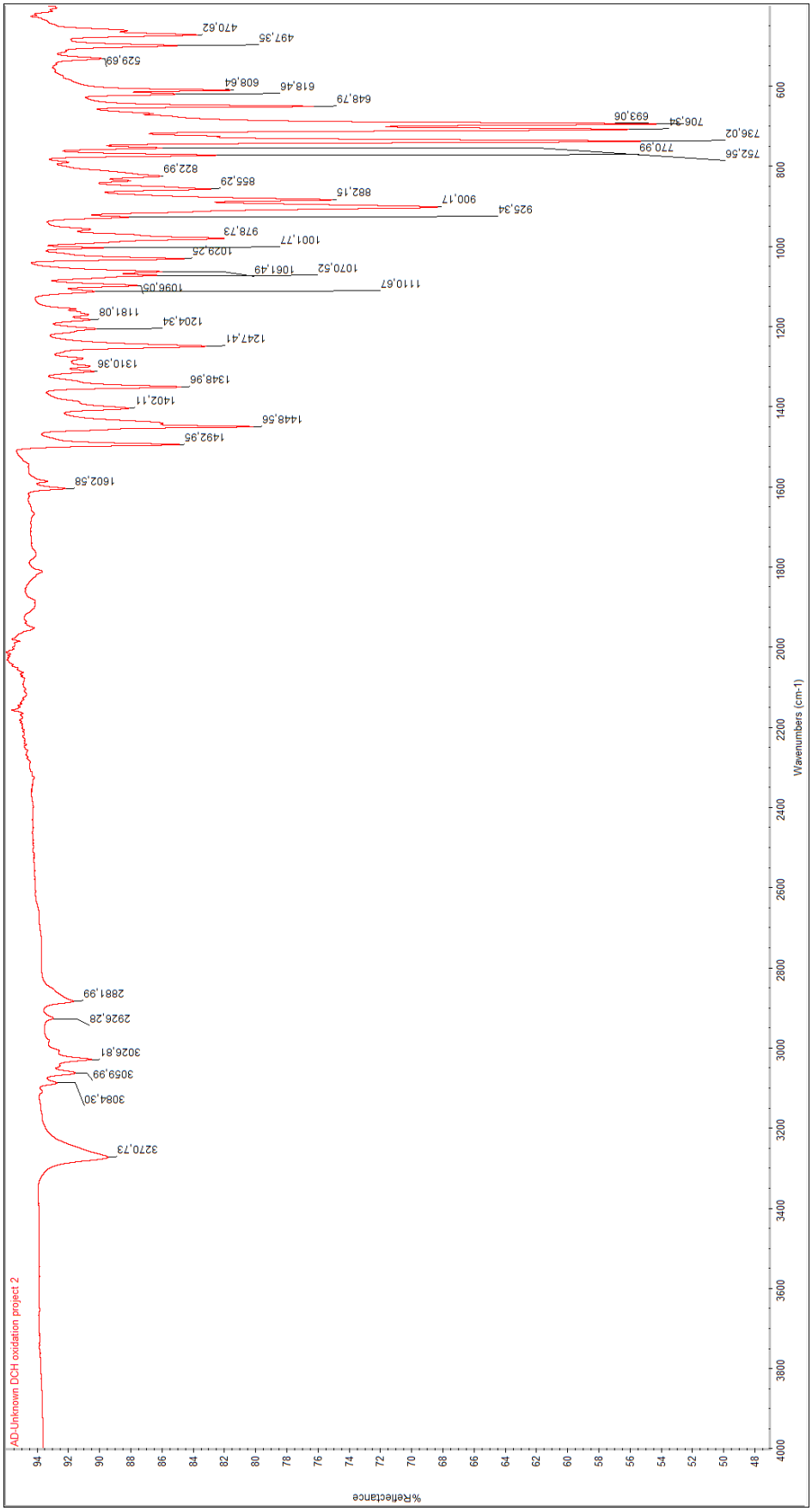

[1] D.O. Cicero, G. Barbato and R. Bazzo, *J. Magn. Reson*. **2001**, *148*, 209-213.

## (2R,4R)-2,4,6-triphenyl-1,3,5-triazabicyclo[3.1.0]hexane (5a): NOESY (600 MHz), DMSO.

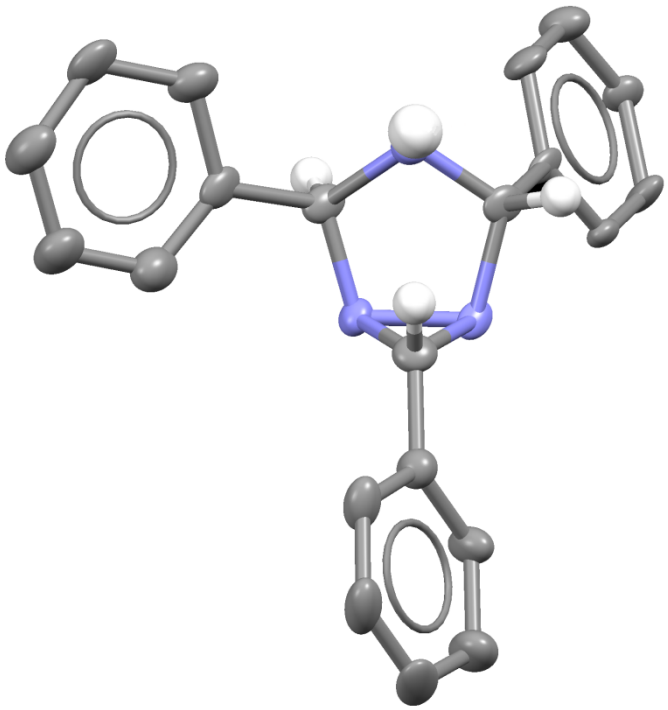
## (2R,4R)-2,4,6-triphenyl-1,3,5-triazabicyclo[3.1.0]hexane (5a) + (2R,4S)-2,4,6-triphenyl-1,3,5-triazabicyclo[3.1.0]hexane (5b): $^{1}$H-NMR in $CDCl_3$



## (2R,4R)-2,4,6-triphenyl-1,3,5-triazabicyclo[3.1.0]hexane (5a): FT-IR



## (2R,4R)-2,4,6-triphenyl-1,3,5-triazabicyclo[3.1.0]hexane (5a): X- Ray crystallography



### Table 1. Crystal data and structure refinement for (5a).

| | | |
|---|---|---|
| Identification code | AD413 | |
| Empirical formula | C21 H19 N3 | |
| Formula weight | 313.39 | |
| Temperature | 293(2) K | |
| Wavelength | 0.72179 Å | |
| Crystal system | Orthorhombic | |
| Space group | $P2_12_12_1$ | |
| Unit cell dimensions | a = 4.54030(10) Å | α= 90°. |
| | b = 20.7027(9) Å | β= 90°. |
| | c = 17.5506(7) Å | γ = 90°. |
| Volume | 1649.69(10) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.262 $Mg/m^3$ | |
| Absorption coefficient | 0.077 $mm^{-1}$ | |
| F(000) | 664 | |
| Crystal size | ? x ? x ? $mm^3$ | |
| Theta range for data collection | 1.545 to 25.442°. | |
| Index ranges | -5<=h<=5, -24<=k<=24, -20<=l<=20 | |
| Reflections collected | 6862 | |
| Independent reflections | 6862 [R(int) = ?] | |
| Completeness to theta = 25.442° | 93.7 % | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 6862 / 195 / 217 | |
| Goodness-of-fit on $F^2$ | 1.129 | |
| Final R indices [I>2sigma(I)] | R1 = 0.1328, wR2 = 0.2786 | |
| R indices (all data) | R1 = 0.1868, wR2 = 0.3056 | |
| Absolute structure parameter | 0.5 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.645 and -0.291 e.$Å^{-3}$ | |

## Table 2. Bond lengths [Å] and angles [°] for (5a).

| | |
|---|---|
| N(1)-C(3) | 1.487(16) |
| N(1)-N(2) | 1.493(14) |
| N(1)-C(1) | 1.514(16) |
| N(2)-C(1) | 1.438(16) |
| N(2)-C(2) | 1.504(16) |
| N(3)-C(2) | 1.446(16) |
| N(3)-C(3) | 1.457(18) |
| N(3)-H(3N) | 1.083(11) |
| C(1)-C(4) | 1.498(17) |
| C(1)-H(1) | 0.9800 |
| C(2)-C(10) | 1.523(18) |
| C(2)-H(2) | 0.9800 |
| C(3)-C(16) | 1.536(19) |
| C(3)-H(3) | 0.9800 |
| C(4)-C(9) | 1.399(18) |
| C(4)-C(5) | 1.408(18) |
| C(5)-C(6) | 1.381(18) |
| C(5)-H(5) | 0.9300 |
| C(6)-C(7) | 1.41(2) |
| C(6)-H(6) | 0.9300 |
| C(7)-C(8) | 1.39(2) |
| C(7)-H(7) | 0.9300 |
| C(8)-C(9) | 1.34(2) |
| C(8)-H(8) | 0.9300 |
| C(9)-H(9) | 0.9300 |
| C(10)-C(11) | 1.385(17) |
| C(10)-C(15) | 1.386(18) |
| C(11)-C(12) | 1.392(19) |
| C(11)-H(11) | 0.9300 |
| C(12)-C(13) | 1.391(19) |
| C(12)-H(12) | 0.9300 |
| C(13)-C(14) | 1.362(16) |
| C(13)-H(13) | 0.9300 |
| C(14)-C(15) | 1.395(18) |
| C(14)-H(14) | 0.9300 |
| C(15)-H(15) | 0.9300 |
| C(16)-C(17) | 1.35(2) |
| C(16)-C(21) | 1.408(19) |
| C(17)-C(18) | 1.37(2) |
| C(17)-H(17) | 0.9300 |
| C(18)-C(19) | 1.36(2) |
| C(18)-H(18) | 0.9300 |
| C(19)-C(20) | 1.36(2) |
| C(19)-H(19) | 0.9300 |
| C(20)-C(21) | 1.444(19) |
| C(20)-H(20) | 0.9300 |
| C(21)-H(21) | 0.9300 |
| | |
| C(3)-N(1)-N(2) | 106.9(10) |
| C(3)-N(1)-C(1) | 111.7(10) |
| N(2)-N(1)-C(1) | 57.1(7) |
| C(1)-N(2)-N(1) | 62.2(7) |
| C(1)-N(2)-C(2) | 111.1(10) |
| N(1)-N(2)-C(2) | 102.9(9) |
| C(2)-N(3)-C(3) | 102.4(10) |
| C(2)-N(3)-H(3N) | 111.4(10) |
| C(3)-N(3)-H(3N) | 117.8(11) |
| N(2)-C(1)-C(4) | 118.4(11) |
| N(2)-C(1)-N(1) | 60.7(8) |
| C(4)-C(1)-N(1) | 120.6(11) |
| N(2)-C(1)-H(1) | 115.4 |
| C(4)-C(1)-H(1) | 115.4 |
| N(1)-C(1)-H(1) | 115.4 |

| | |
|---|---|
| N(3)-C(2)-N(2) | 109.7(10) |
| N(3)-C(2)-C(10) | 112.4(10) |
| N(2)-C(2)-C(10) | 109.5(11) |
| N(3)-C(2)-H(2) | 108.3 |
| N(2)-C(2)-H(2) | 108.3 |
| C(10)-C(2)-H(2) | 108.3 |
| N(3)-C(3)-N(1) | 108.1(10) |
| N(3)-C(3)-C(16) | 113.4(11) |
| N(1)-C(3)-C(16) | 113.0(11) |
| N(3)-C(3)-H(3) | 107.3 |
| N(1)-C(3)-H(3) | 107.3 |
| C(16)-C(3)-H(3) | 107.3 |
| C(9)-C(4)-C(5) | 117.9(13) |
| C(9)-C(4)-C(1) | 119.8(12) |
| C(5)-C(4)-C(1) | 122.3(12) |
| C(6)-C(5)-C(4) | 121.2(13) |
| C(6)-C(5)-H(5) | 119.4 |
| C(4)-C(5)-H(5) | 119.4 |
| C(5)-C(6)-C(7) | 119.2(15) |
| C(5)-C(6)-H(6) | 120.4 |
| C(7)-C(6)-H(6) | 120.4 |
| C(8)-C(7)-C(6) | 118.9(14) |
| C(8)-C(7)-H(7) | 120.6 |
| C(6)-C(7)-H(7) | 120.6 |
| C(9)-C(8)-C(7) | 121.7(15) |
| C(9)-C(8)-H(8) | 119.1 |
| C(7)-C(8)-H(8) | 119.1 |
| C(8)-C(9)-C(4) | 121.1(15) |
| C(8)-C(9)-H(9) | 119.5 |
| C(4)-C(9)-H(9) | 119.5 |
| C(11)-C(10)-C(15) | 119.1(12) |
| C(11)-C(10)-C(2) | 120.6(12) |
| C(15)-C(10)-C(2) | 120.3(11) |
| C(10)-C(11)-C(12) | 121.9(13) |
| C(10)-C(11)-H(11) | 119.0 |
| C(12)-C(11)-H(11) | 119.0 |
| C(13)-C(12)-C(11) | 117.8(13) |
| C(13)-C(12)-H(12) | 121.1 |
| C(11)-C(12)-H(12) | 121.1 |
| C(14)-C(13)-C(12) | 120.8(13) |
| C(14)-C(13)-H(13) | 119.6 |
| C(12)-C(13)-H(13) | 119.6 |
| C(13)-C(14)-C(15) | 121.2(13) |
| C(13)-C(14)-H(14) | 119.4 |
| C(15)-C(14)-H(14) | 119.4 |
| C(10)-C(15)-C(14) | 119.1(12) |
| C(10)-C(15)-H(15) | 120.5 |
| C(14)-C(15)-H(15) | 120.5 |
| C(17)-C(16)-C(21) | 121.1(13) |
| C(17)-C(16)-C(3) | 122.0(13) |
| C(21)-C(16)-C(3) | 116.8(13) |
| C(16)-C(17)-C(18) | 120.1(15) |
| C(16)-C(17)-H(17) | 119.9 |
| C(18)-C(17)-H(17) | 119.9 |
| C(19)-C(18)-C(17) | 120.0(16) |
| C(19)-C(18)-H(18) | 120.0 |
| C(17)-C(18)-H(18) | 120.0 |
| C(20)-C(19)-C(18) | 123.6(15) |
| C(20)-C(19)-H(19) | 118.2 |
| C(18)-C(19)-H(19) | 118.2 |
| C(19)-C(20)-C(21) | 116.5(14) |
| C(19)-C(20)-H(20) | 121.8 |
| C(21)-C(20)-H(20) | 121.8 |
| C(16)-C(21)-C(20) | 118.7(14) |
| C(16)-C(21)-H(21) | 120.6 |

| | |
|---|---|
| C(20)-C(21)-H(21) | 120.6 |

Symmetry transformations used to generate equivalent atoms:

## Table 3. Torsion angles [°] for (5a).

| | |
|---|---|
| C(3)-N(1)-N(2)-C(1) | 105.3(10) |
| C(3)-N(1)-N(2)-C(2) | -2.0(12) |
| C(1)-N(1)-N(2)-C(2) | -107.2(10) |
| N(1)-N(2)-C(1)-C(4) | 111.1(13) |
| C(2)-N(2)-C(1)-C(4) | -155.1(11) |
| C(2)-N(2)-C(1)-N(1) | 93.9(10) |
| C(3)-N(1)-C(1)-N(2) | -96.7(11) |
| C(3)-N(1)-C(1)-C(4) | 155.8(11) |
| N(2)-N(1)-C(1)-C(4) | -107.5(14) |
| C(3)-N(3)-C(2)-N(2) | -31.4(12) |
| C(3)-N(3)-C(2)-C(10) | 90.8(12) |
| C(1)-N(2)-C(2)-N(3) | -43.9(13) |
| N(1)-N(2)-C(2)-N(3) | 21.0(12) |
| C(1)-N(2)-C(2)-C(10) | -167.7(10) |
| N(1)-N(2)-C(2)-C(10) | -102.9(11) |
| C(2)-N(3)-C(3)-N(1) | 29.4(13) |
| C(2)-N(3)-C(3)-C(16) | 155.6(11) |
| N(2)-N(1)-C(3)-N(3) | -17.3(13) |
| C(1)-N(1)-C(3)-N(3) | 43.4(14) |
| N(2)-N(1)-C(3)-C(16) | -143.6(10) |
| C(1)-N(1)-C(3)-C(16) | -82.9(13) |
| N(2)-C(1)-C(4)-C(9) | 178.4(12) |
| N(1)-C(1)-C(4)-C(9) | -110.7(15) |
| N(2)-C(1)-C(4)-C(5) | -3(2) |
| N(1)-C(1)-C(4)-C(5) | 67.5(19) |
| C(9)-C(4)-C(5)-C(6) | -3(2) |
| C(1)-C(4)-C(5)-C(6) | 178.9(14) |
| C(4)-C(5)-C(6)-C(7) | 3(2) |
| C(5)-C(6)-C(7)-C(8) | -2(2) |
| C(6)-C(7)-C(8)-C(9) | 1(2) |
| C(7)-C(8)-C(9)-C(4) | -1(2) |
| C(5)-C(4)-C(9)-C(8) | 2(2) |
| C(1)-C(4)-C(9)-C(8) | -179.7(14) |
| N(3)-C(2)-C(10)-C(11) | 24.1(18) |
| N(2)-C(2)-C(10)-C(11) | 146.4(12) |
| N(3)-C(2)-C(10)-C(15) | -157.1(12) |
| N(2)-C(2)-C(10)-C(15) | -34.8(16) |
| C(15)-C(10)-C(11)-C(12) | -1(2) |
| C(2)-C(10)-C(11)-C(12) | 178.1(13) |
| C(10)-C(11)-C(12)-C(13) | 1(2) |
| C(11)-C(12)-C(13)-C(14) | -2(2) |
| C(12)-C(13)-C(14)-C(15) | 3(2) |
| C(11)-C(10)-C(15)-C(14) | 1.8(19) |
| C(2)-C(10)-C(15)-C(14) | -177.0(13) |
| C(13)-C(14)-C(15)-C(10) | -3(2) |
| N(3)-C(3)-C(16)-C(17) | -137.6(13) |
| N(1)-C(3)-C(16)-C(17) | -14.1(18) |
| N(3)-C(3)-C(16)-C(21) | 45.3(16) |
| N(1)-C(3)-C(16)-C(21) | 168.8(11) |
| C(21)-C(16)-C(17)-C(18) | 0(2) |
| C(3)-C(16)-C(17)-C(18) | -176.4(14) |
| C(16)-C(17)-C(18)-C(19) | 1(2) |
| C(17)-C(18)-C(19)-C(20) | 0(2) |
| C(18)-C(19)-C(20)-C(21) | -1(2) |
| C(17)-C(16)-C(21)-C(20) | -2(2) |
| C(3)-C(16)-C(21)-C(20) | 175.1(13) |
| C(19)-C(20)-C(21)-C(16) | 2(2) |

Symmetry transformations used to generate equivalent atoms: