

# Supporting Information

for

## A practical synthesis of long-chain iso-fatty acids (iso-C<sub>12</sub>–C<sub>19</sub>) and related natural products

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University of Melbourne, Parkville, Victoria 3010, Australia

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### NMR spectra

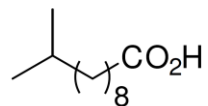
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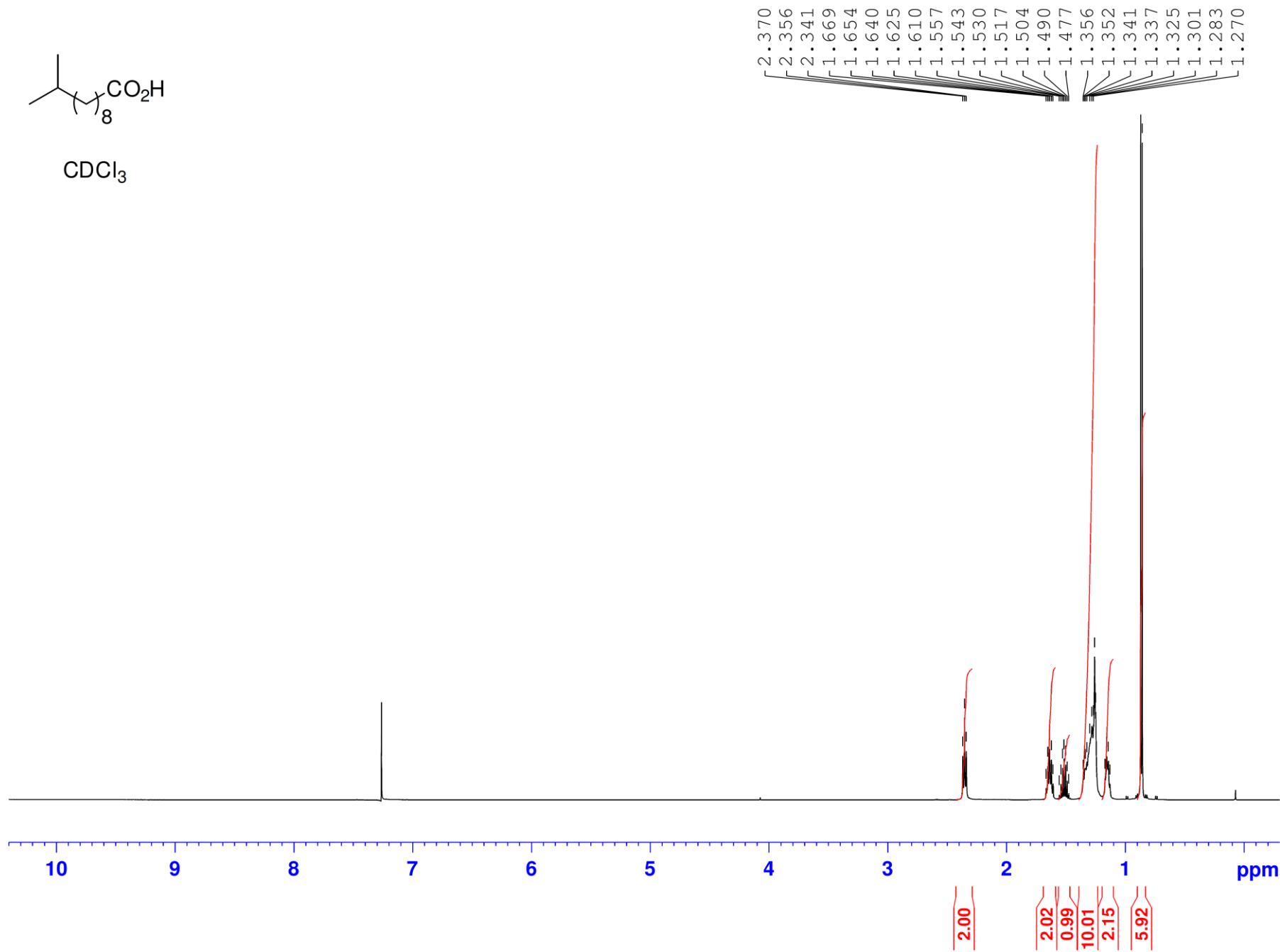
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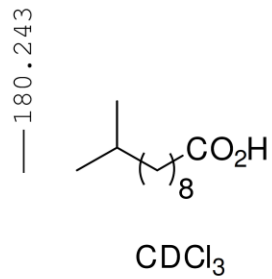
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) – 10-Methylundecanoic acid (**1**)



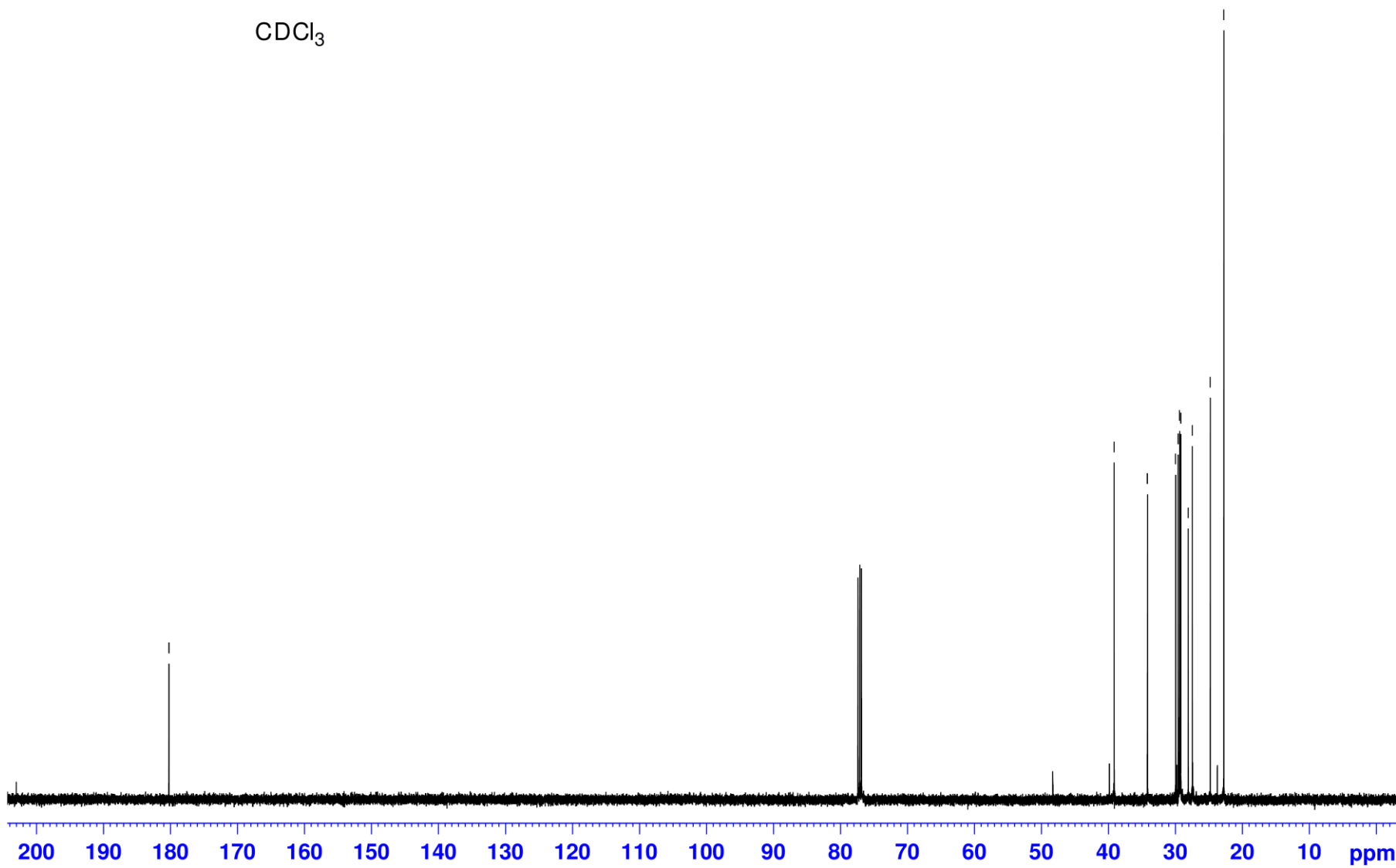
$\text{CDCl}_3$



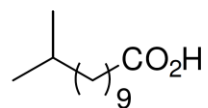
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 10-Methylundecanoic acid (**1**)



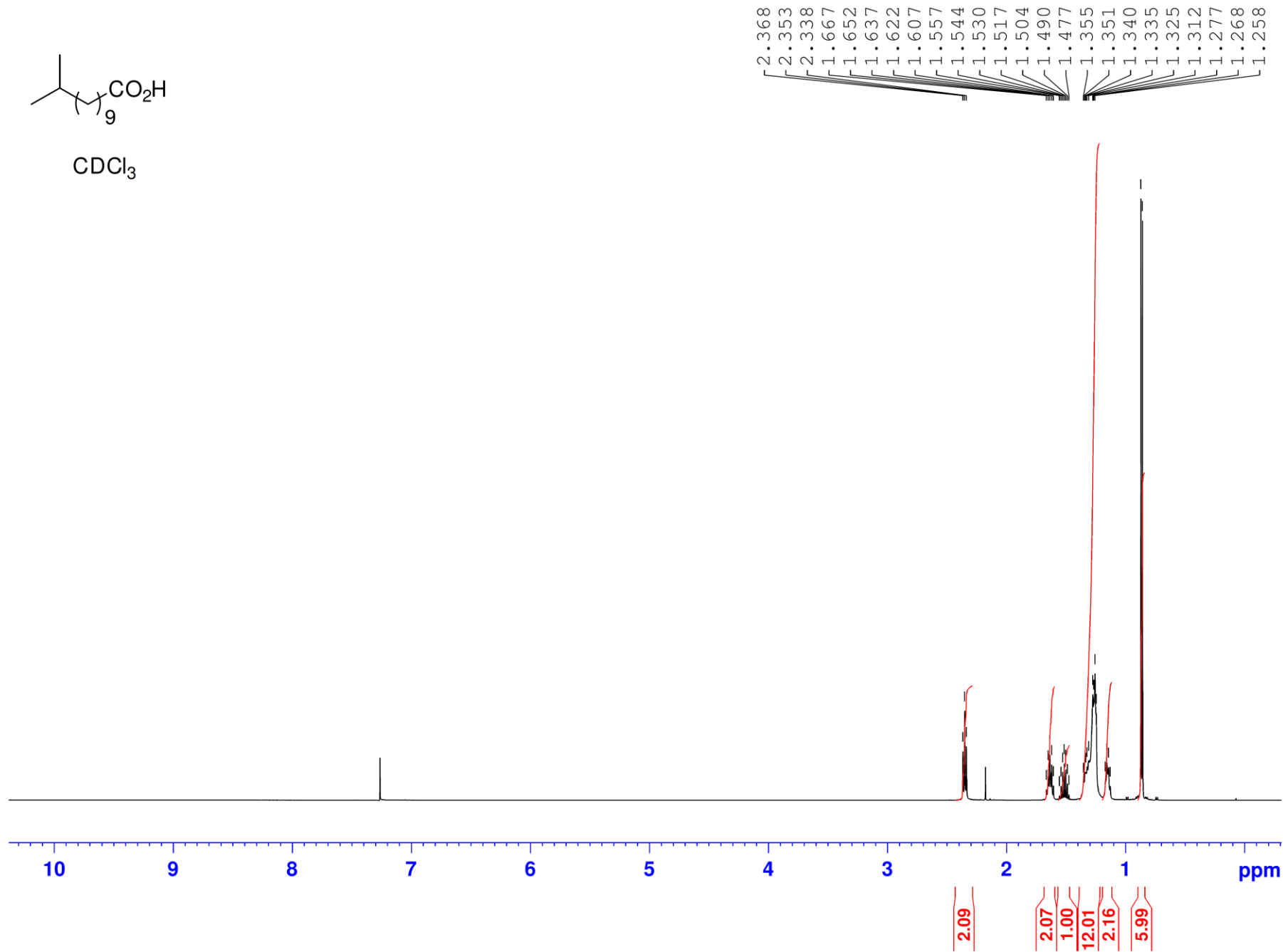
39.174  
34.194  
29.986  
29.608  
29.388  
29.212  
28.110  
27.511  
24.825  
22.799



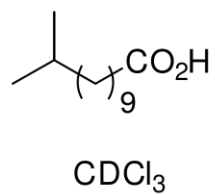
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – 11-Methyldodecanoic acid (**2**)



CDCl<sub>3</sub>

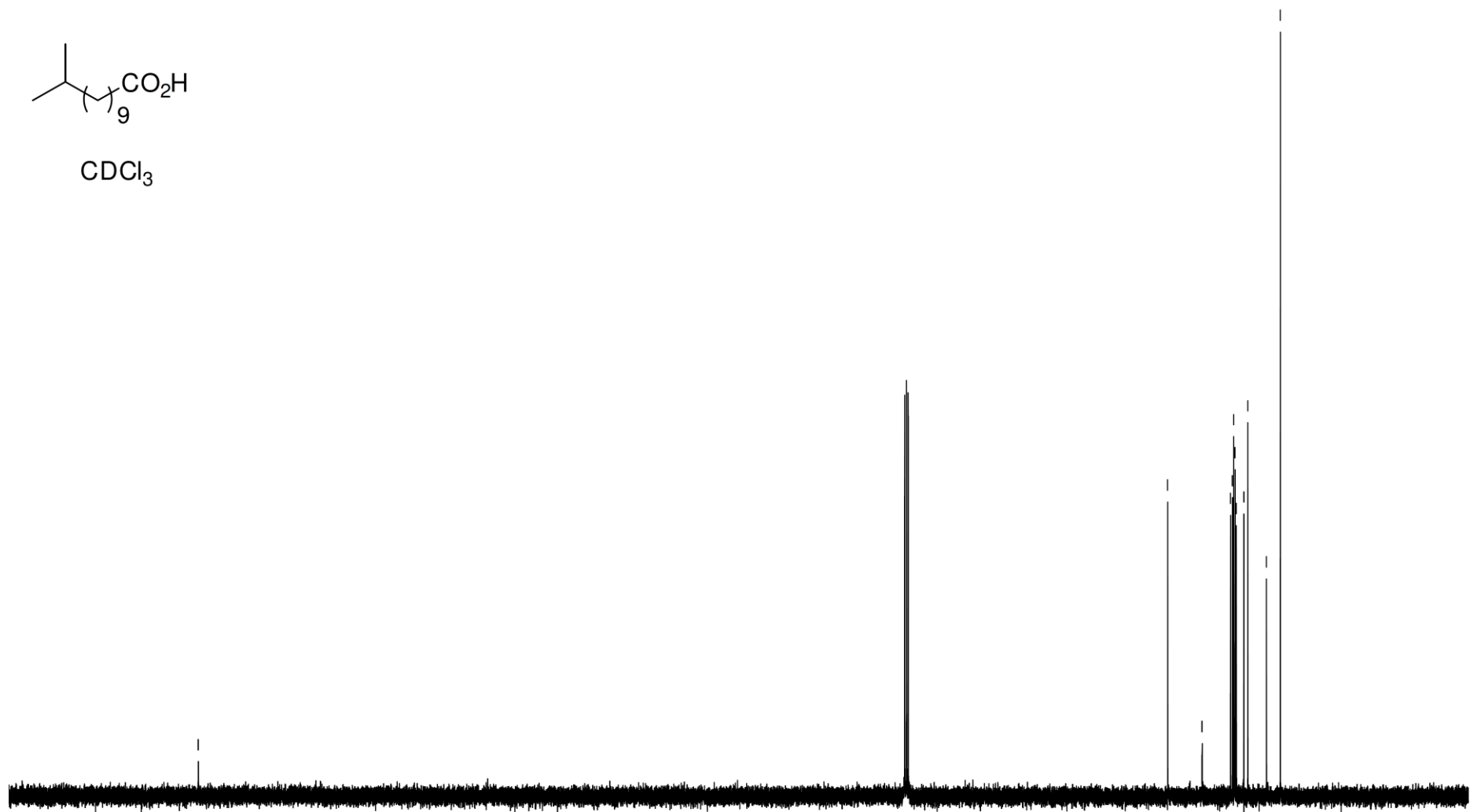


$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 11-Methyldodecanoic acid (**2**)

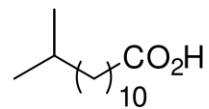


— 180.058

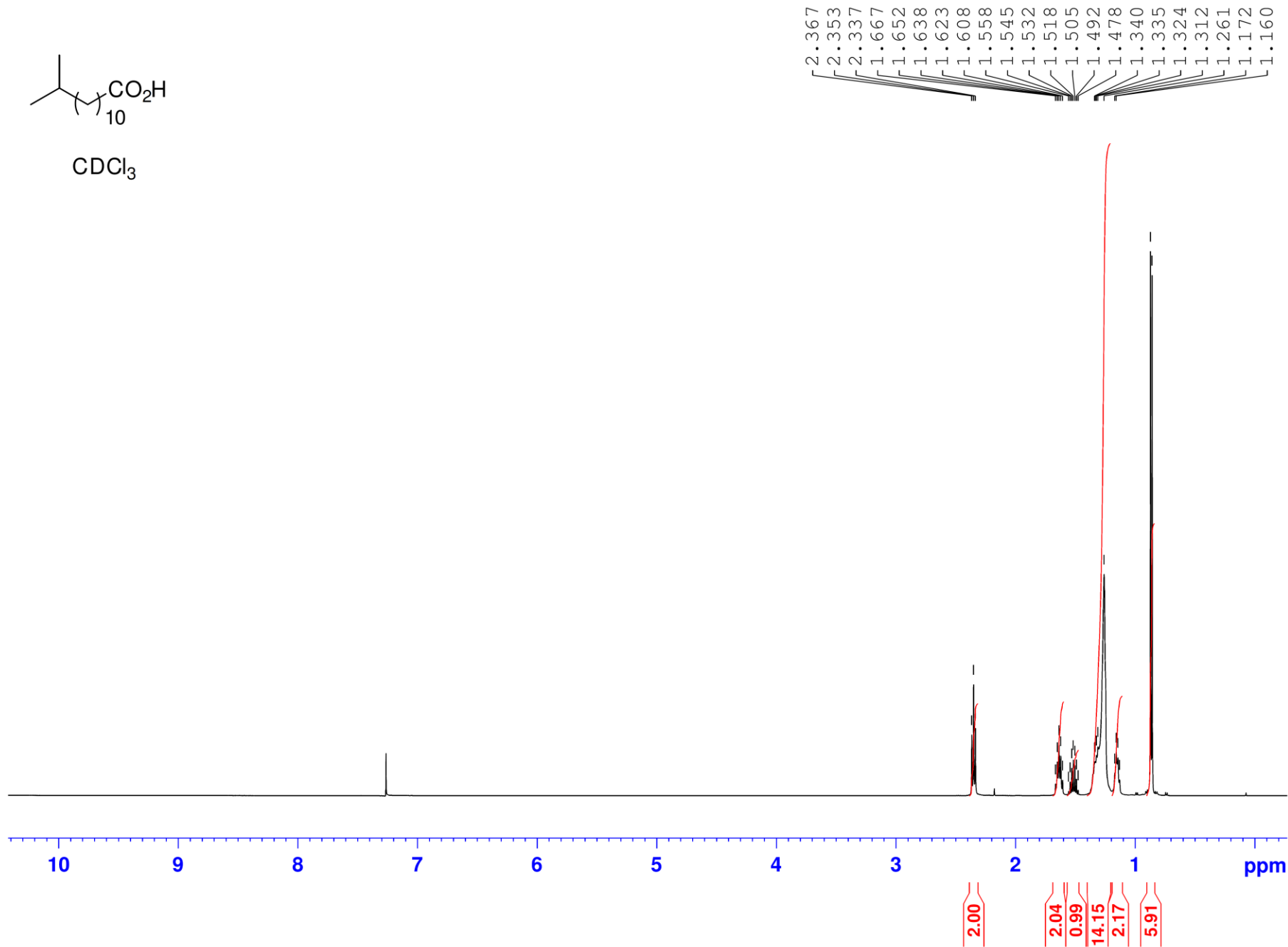
39.196  
34.178  
30.043  
29.770  
29.587  
29.395  
29.212  
28.121  
27.544  
24.837  
22.806



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) – 12-Methyltridecanoic acid (**3**)

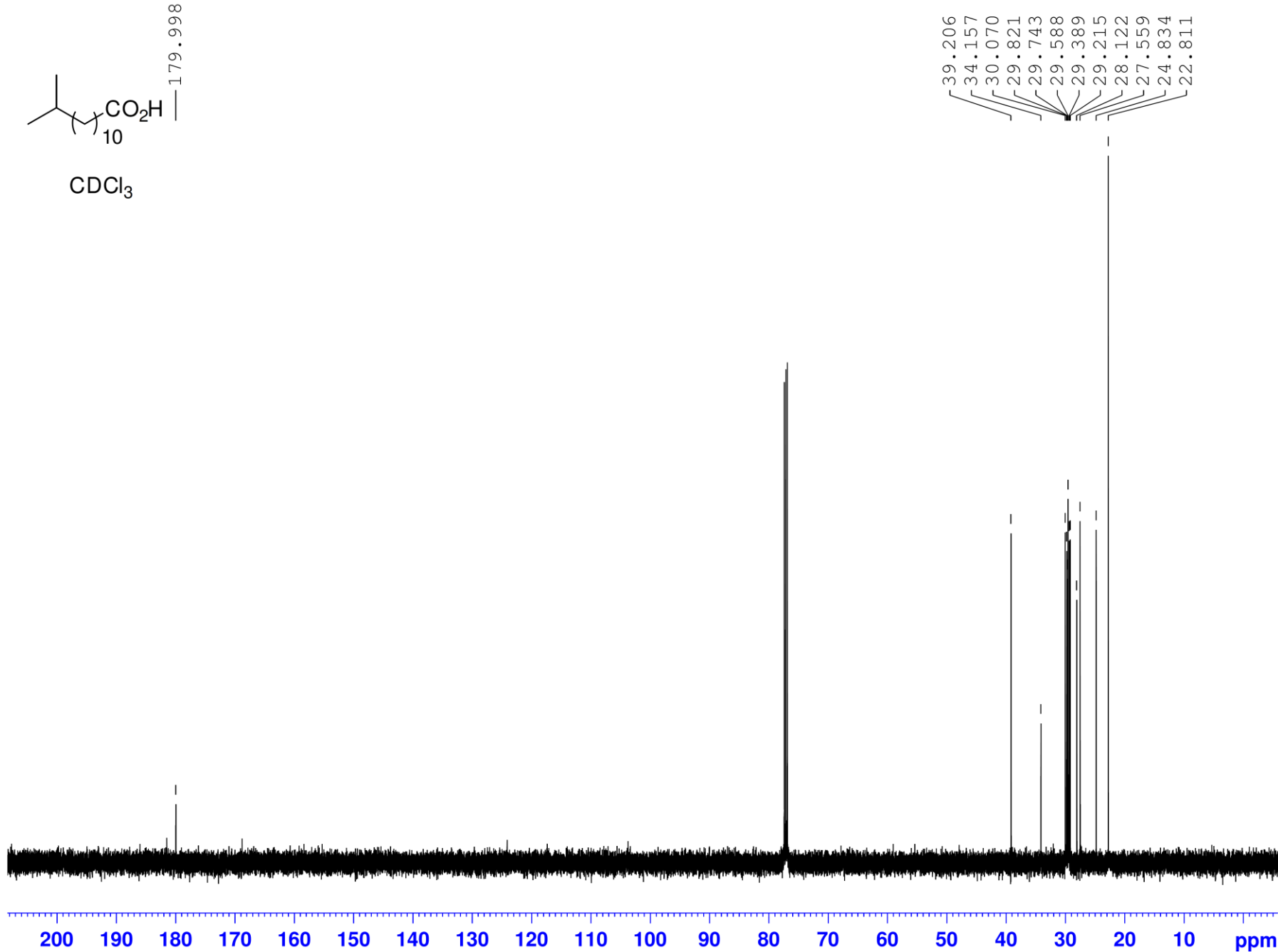
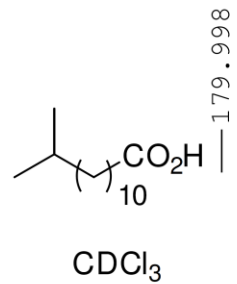


$\text{CDCl}_3$

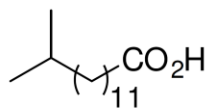




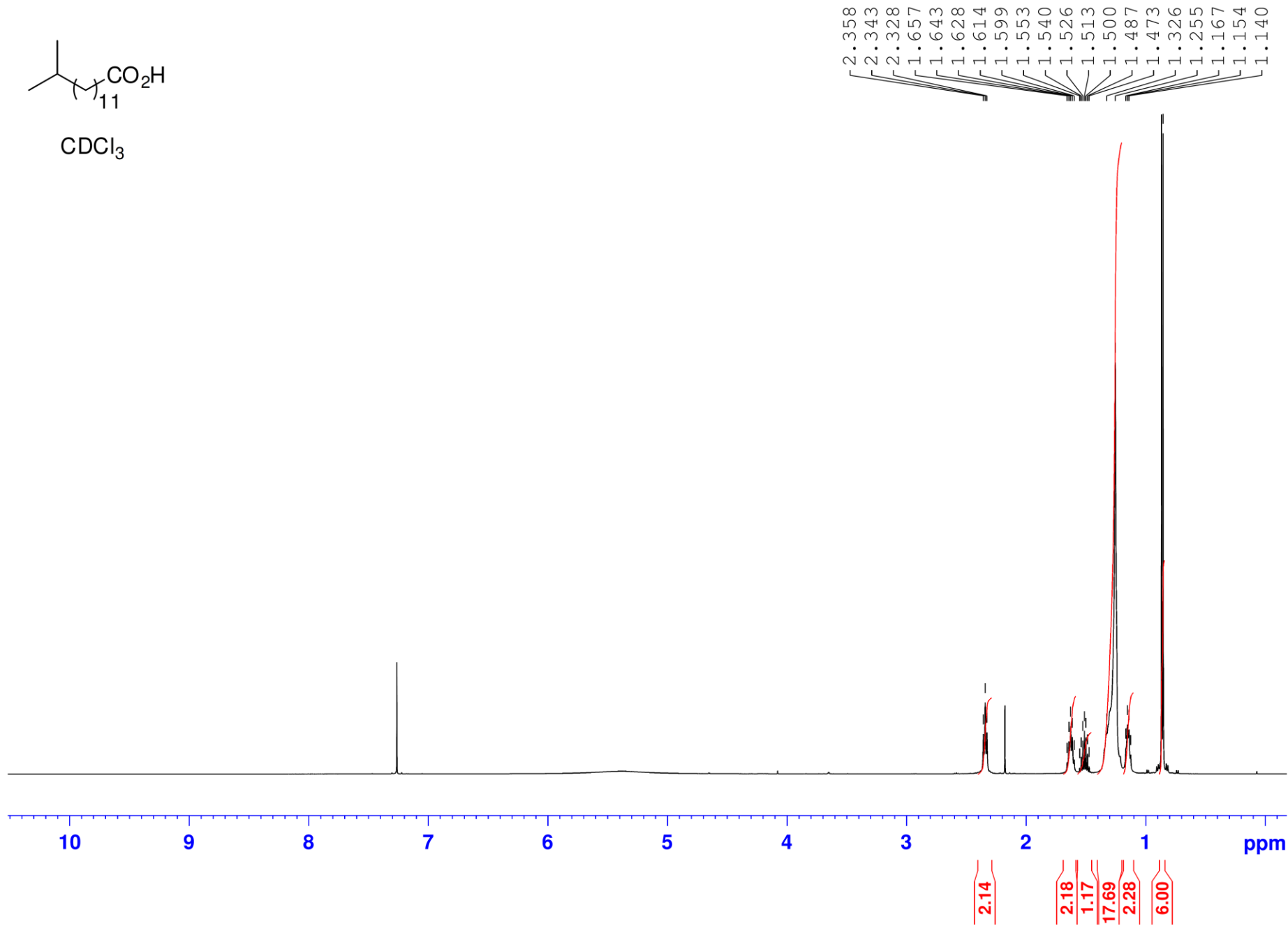
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 12-Methyltridecanoic acid (**3**)



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) – 13-Methyltetradecanoic acid (**4**)

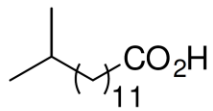


$\text{CDCl}_3$



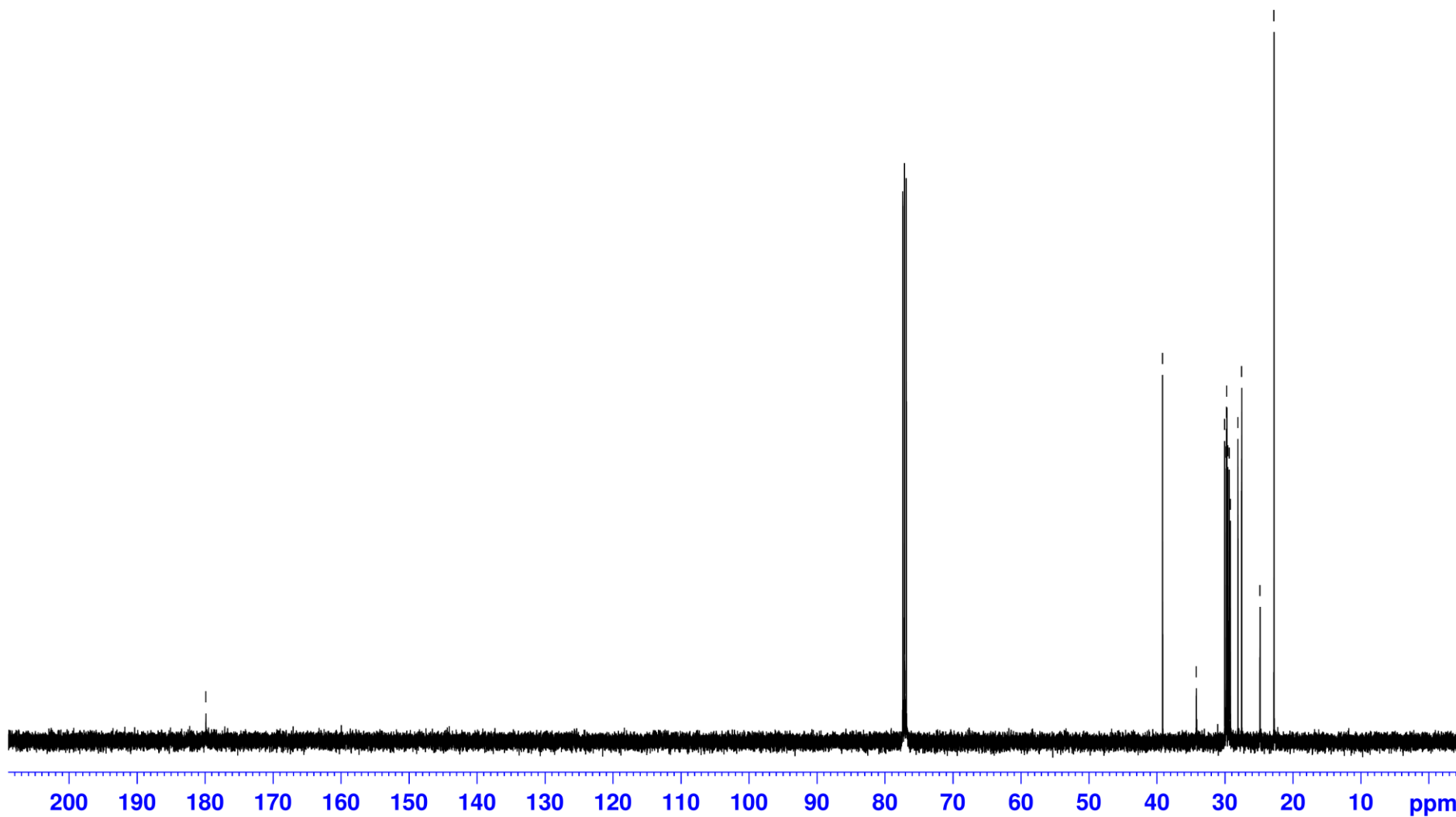
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 13-Methyltetradecanoic acid (**4**)

— 179.892

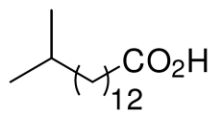


$\text{CDCl}_3$

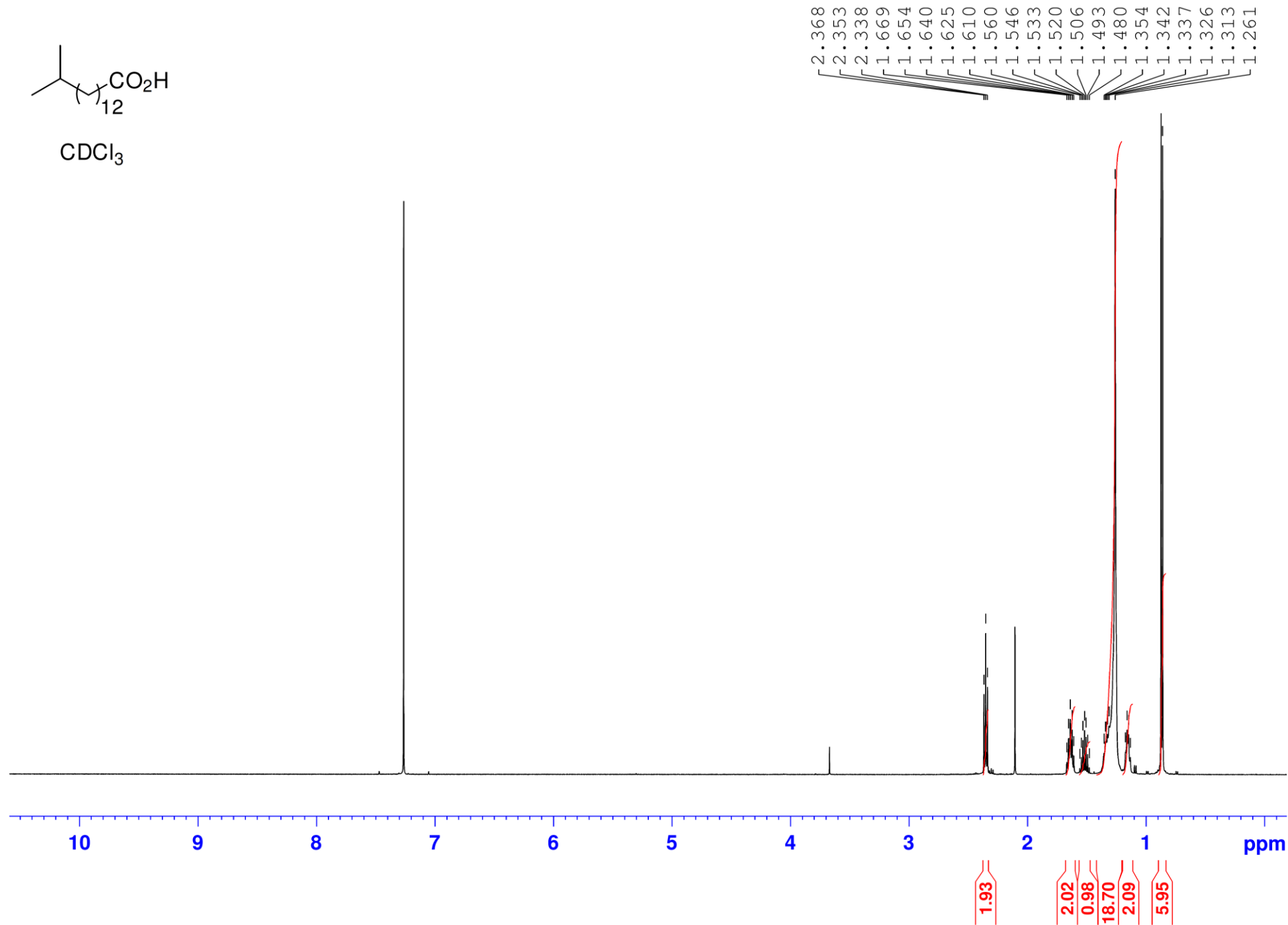
39.197  
34.219  
30.081  
29.849  
29.793  
29.746  
29.586  
29.398  
29.219  
28.113  
27.565  
24.860  
22.809



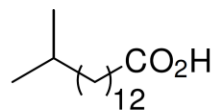
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – 14-Methylpentadecanoic acid (**5**)



CDCl<sub>3</sub>



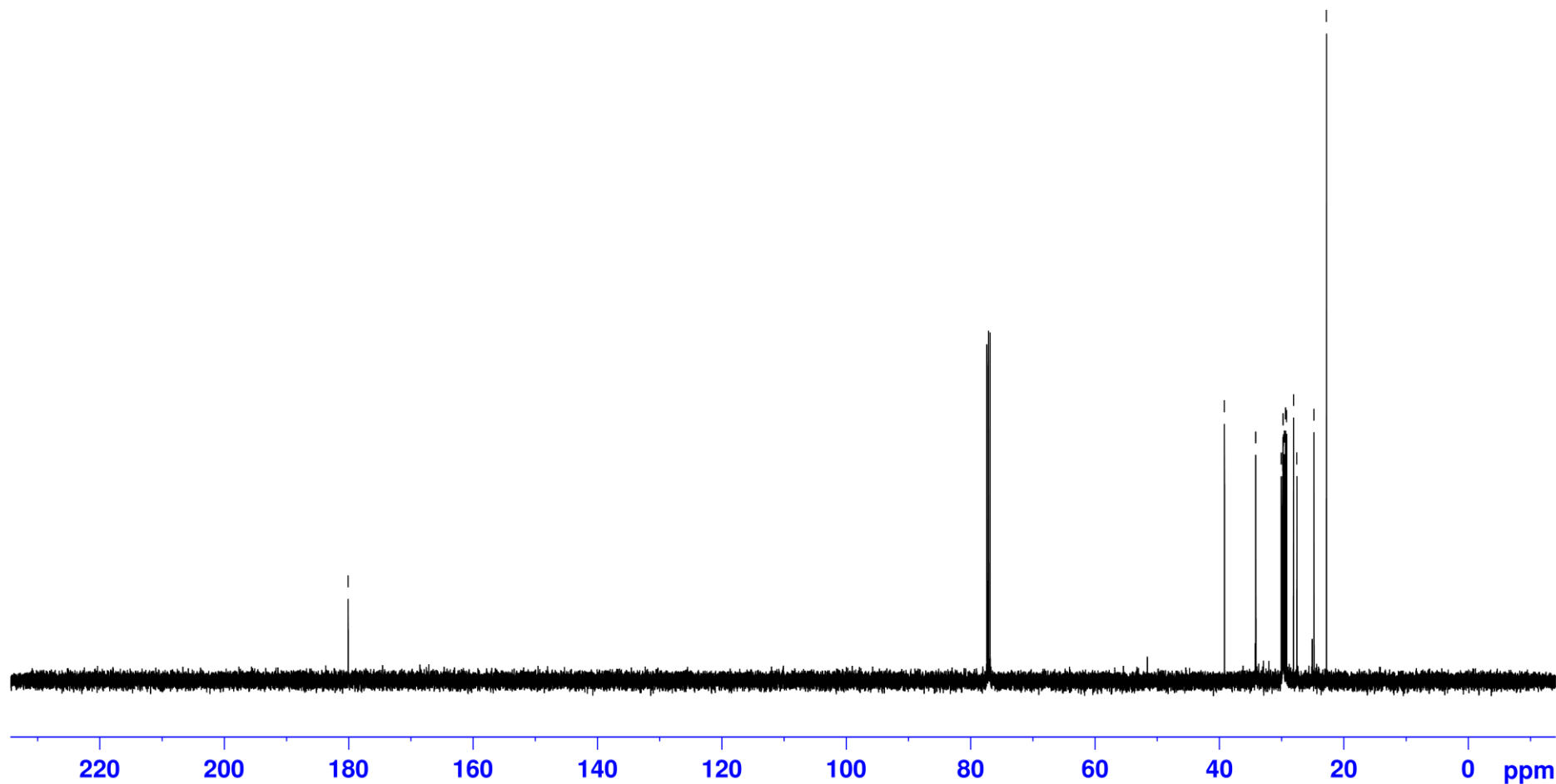
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 14-Methylpentadecanoic acid (**5**)



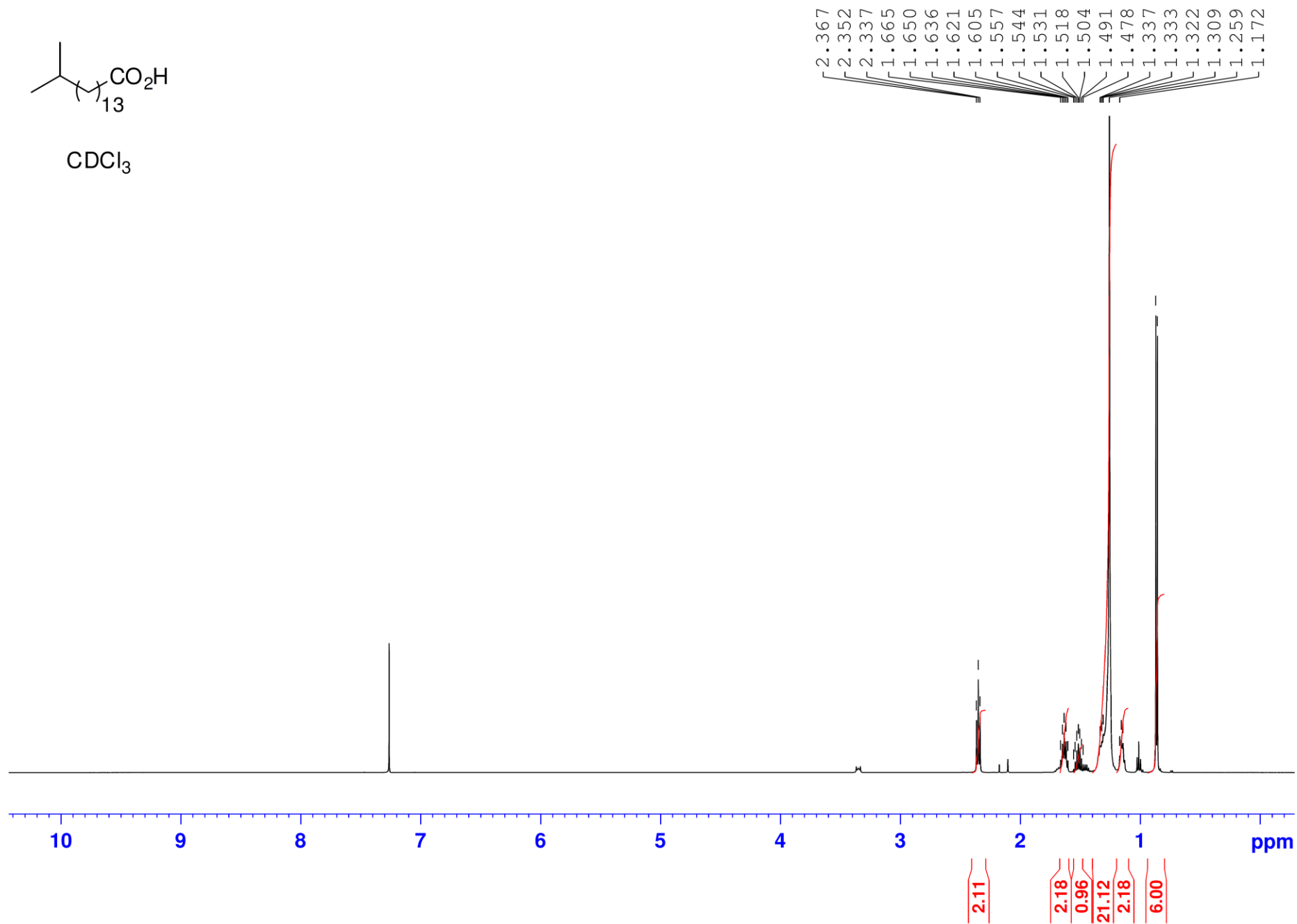
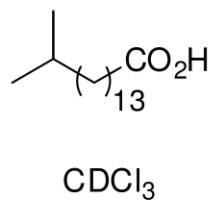
$\text{CDCl}_3$

— 180.117

39.206  
34.171  
30.085  
29.858  
29.812  
29.785  
29.733  
29.577  
29.383  
29.204  
28.115  
27.563  
24.820  
22.803

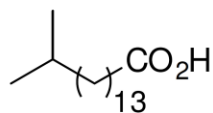


$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) – 15-Methylhexadecanoic acid (**6**)



$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 15-Methylhexadecanoic acid (**6**)

— 179.511



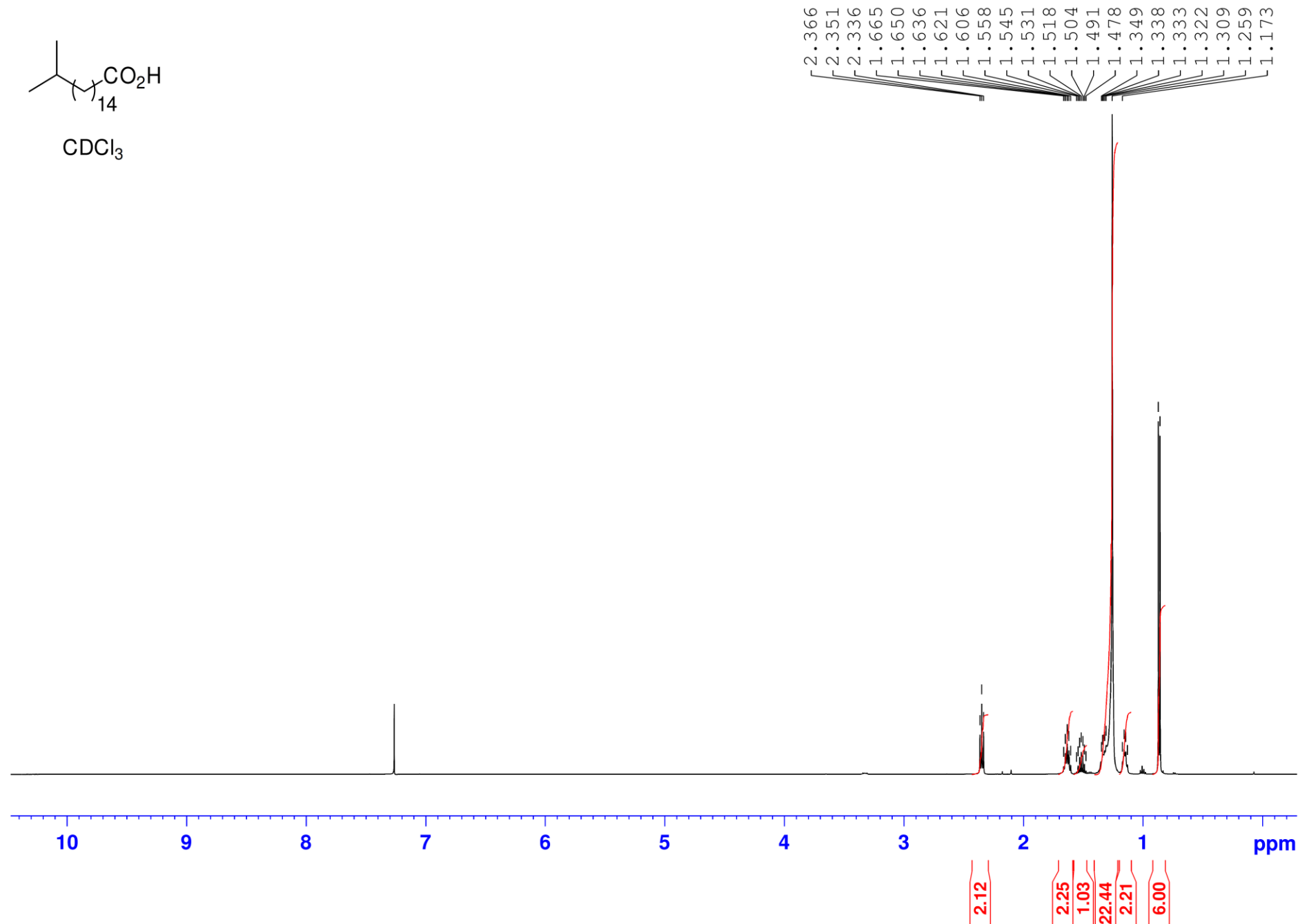
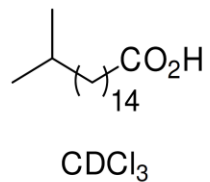
$\text{CDCl}_3$

39.217  
34.135  
30.098  
29.875  
29.837  
29.823  
29.791  
29.744  
29.589  
29.398  
29.223  
28.124  
27.575  
24.861  
22.814



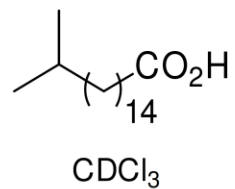
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm S15

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – 16-Methylheptadecanoic acid (**7**)



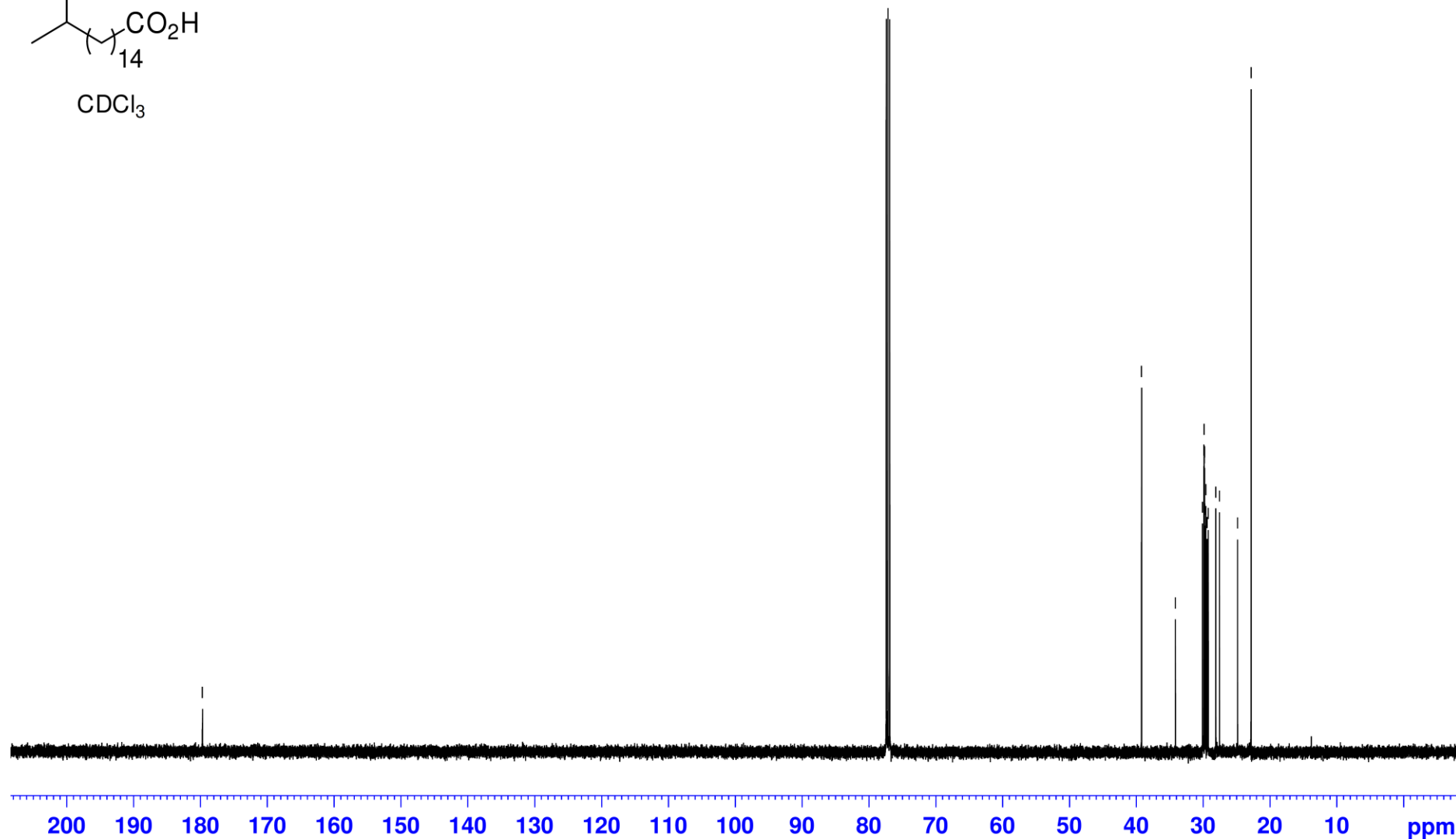


$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 16-Methylheptadecanoic acid (**7**)

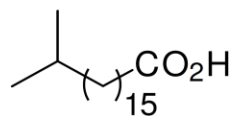


— 179.737

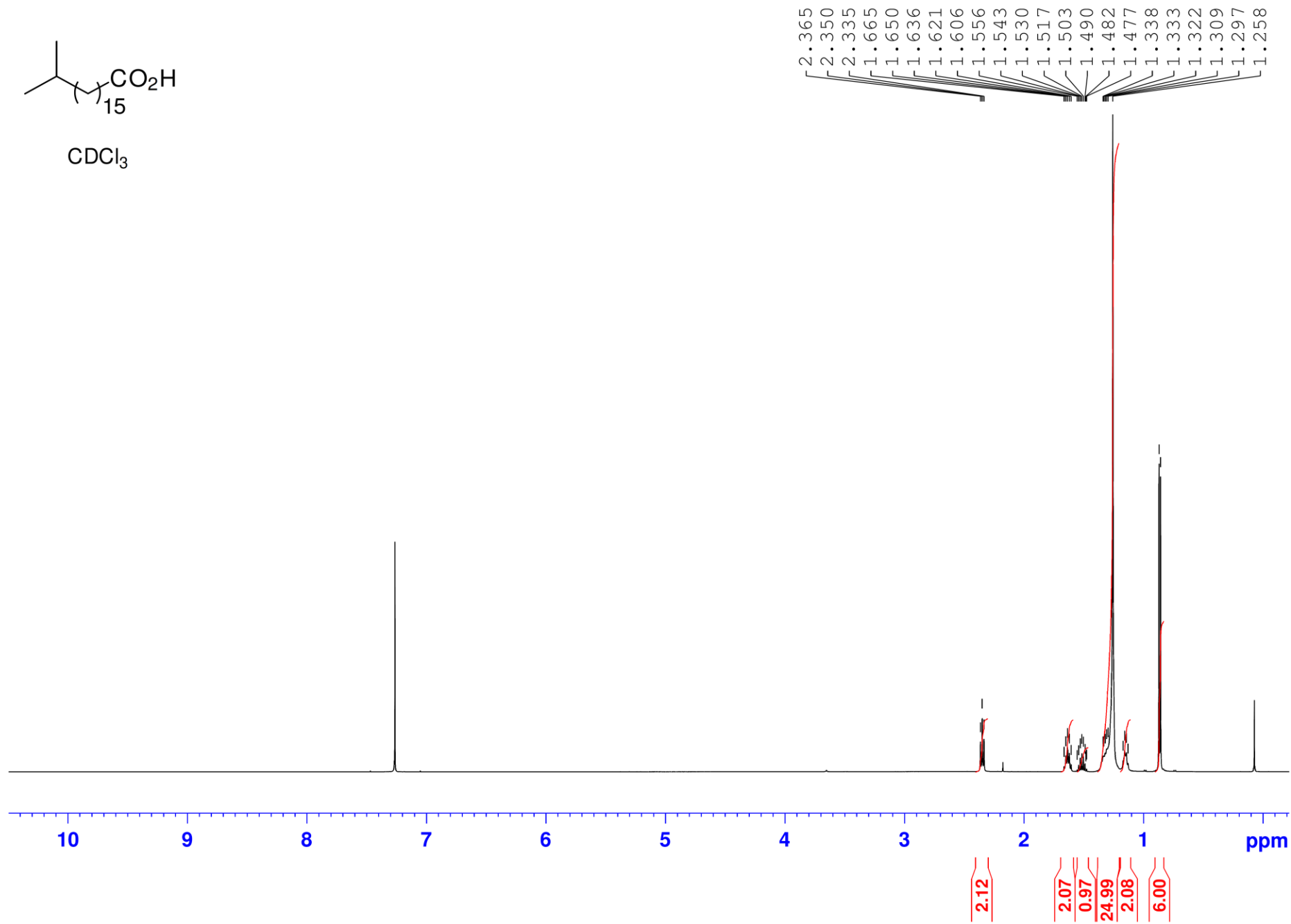
39.221  
34.157  
30.104  
29.881  
29.847  
29.841  
29.820  
29.794  
29.745  
29.592  
29.398  
29.224  
28.125  
27.577  
24.855  
22.815



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) – 17-Methyloctatadecanoic acid (**8**)

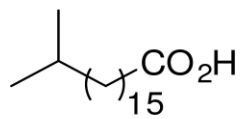


$\text{CDCl}_3$



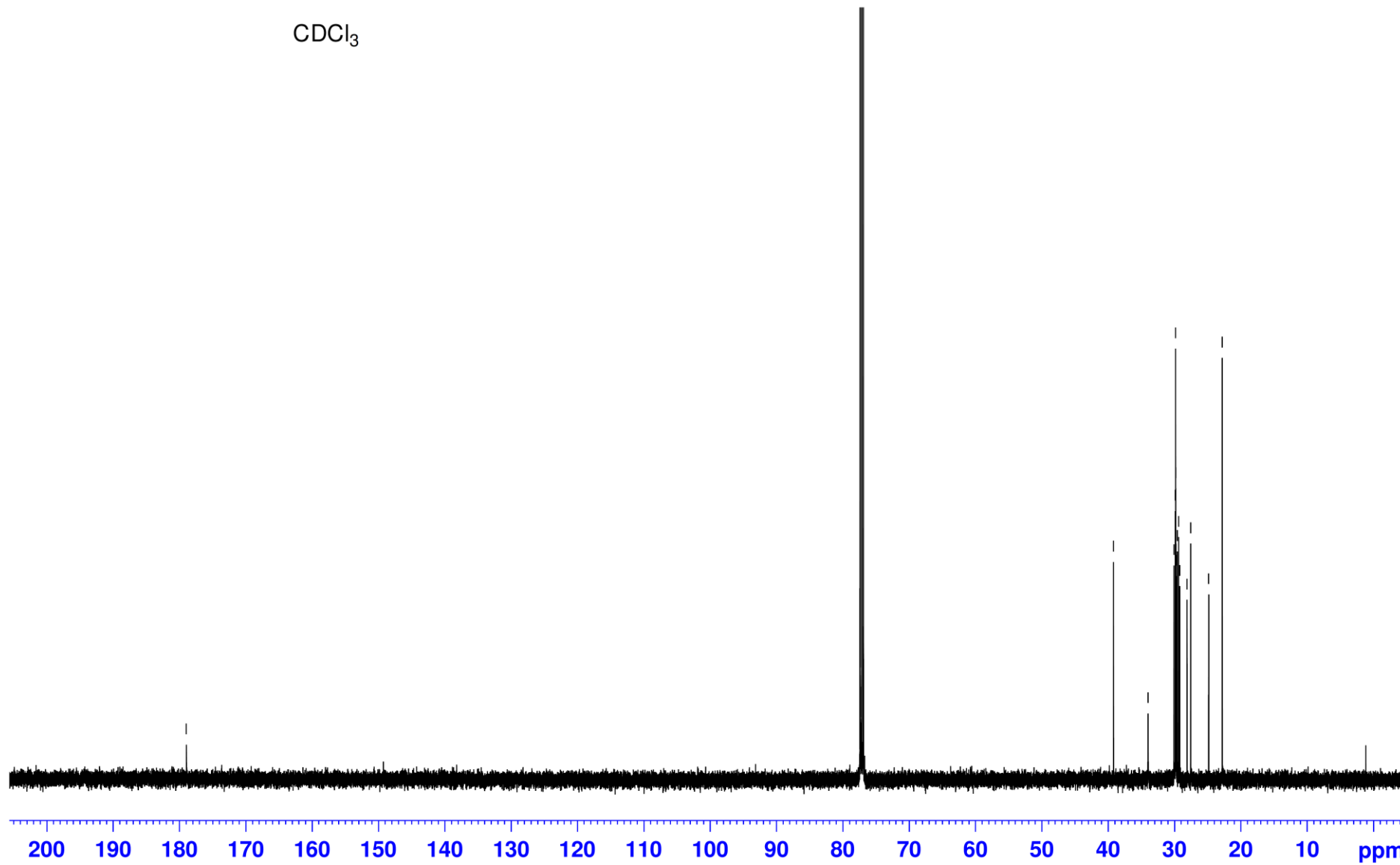
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 17-Methyloctadecanoic acid (**8**)

— 178.982

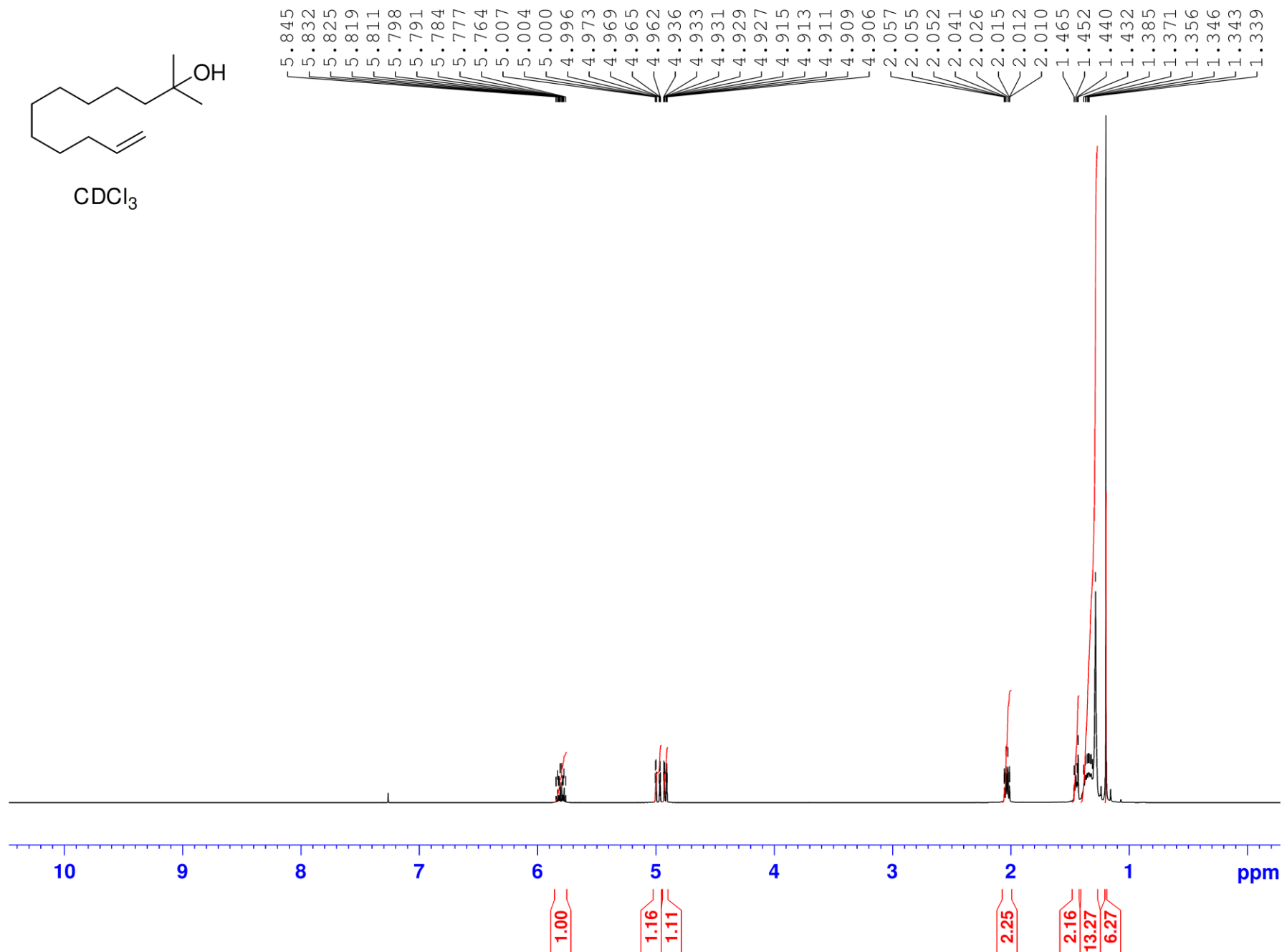
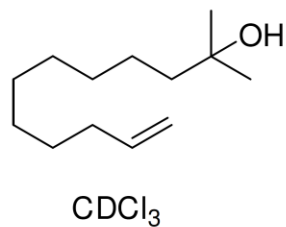


$\text{CDCl}_3$

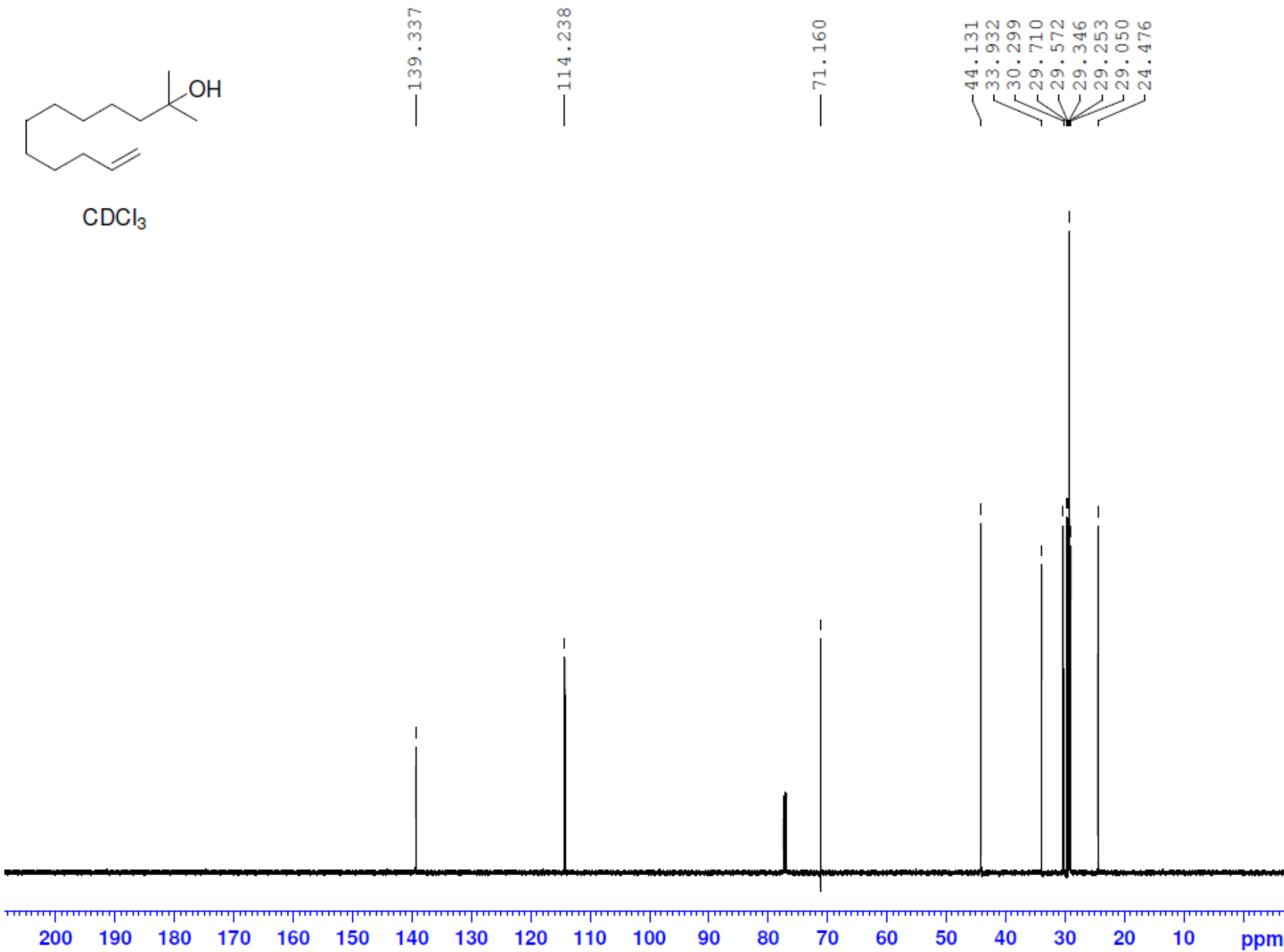
39.215  
34.001  
30.101  
29.881  
29.846  
29.832  
29.820  
29.791  
29.742  
29.588  
29.392  
29.216  
28.122  
27.575  
24.849  
22.814



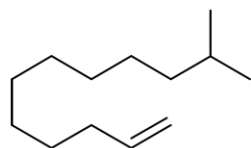
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – 2-Methyldodec-11-en-2-ol (**10**)



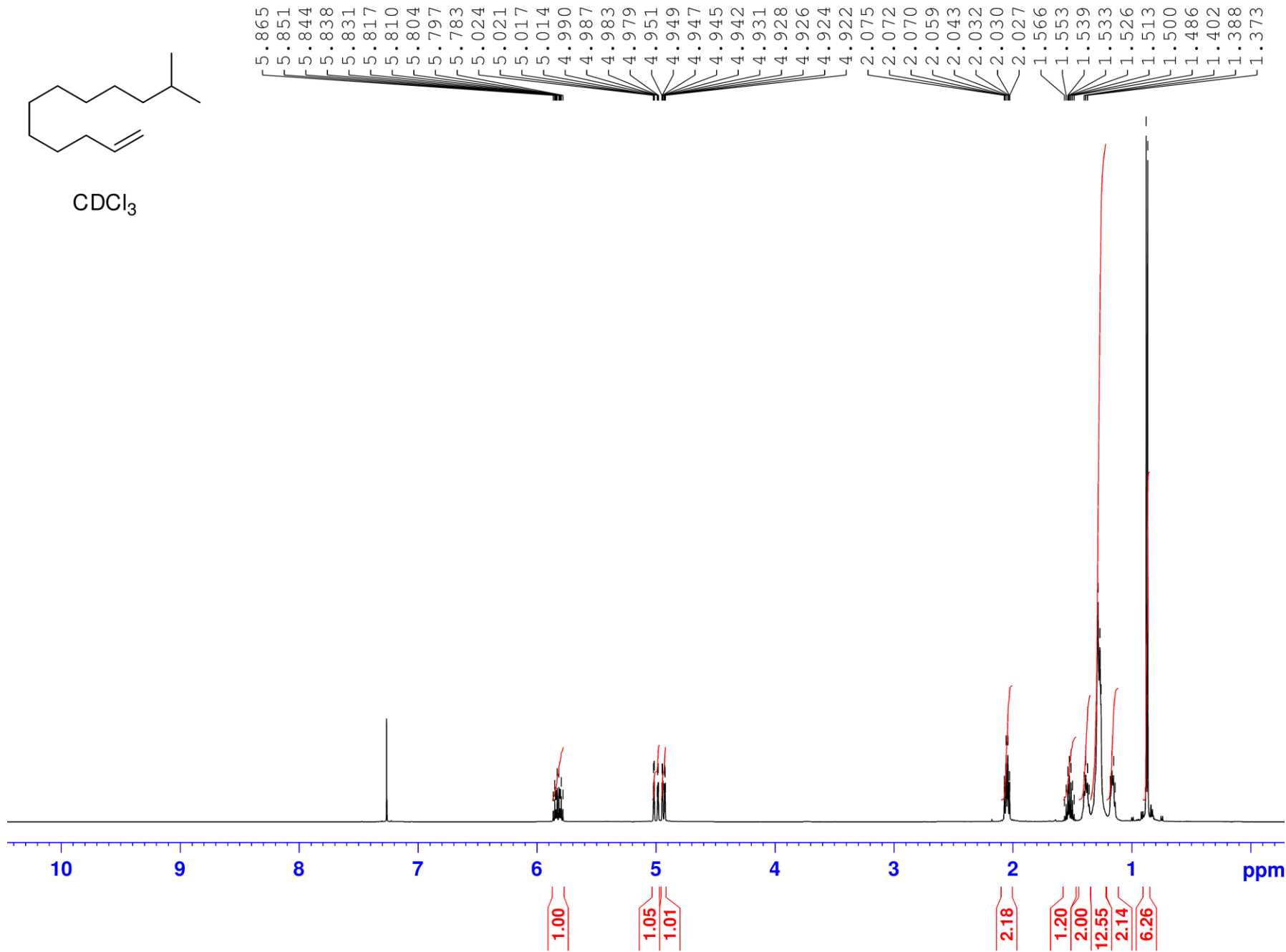
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 2-Methyldodec-11-en-2-ol (**10**)



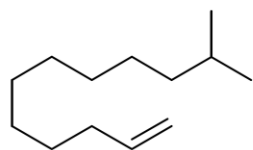
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – 11-Methyldodec-1-ene (11)



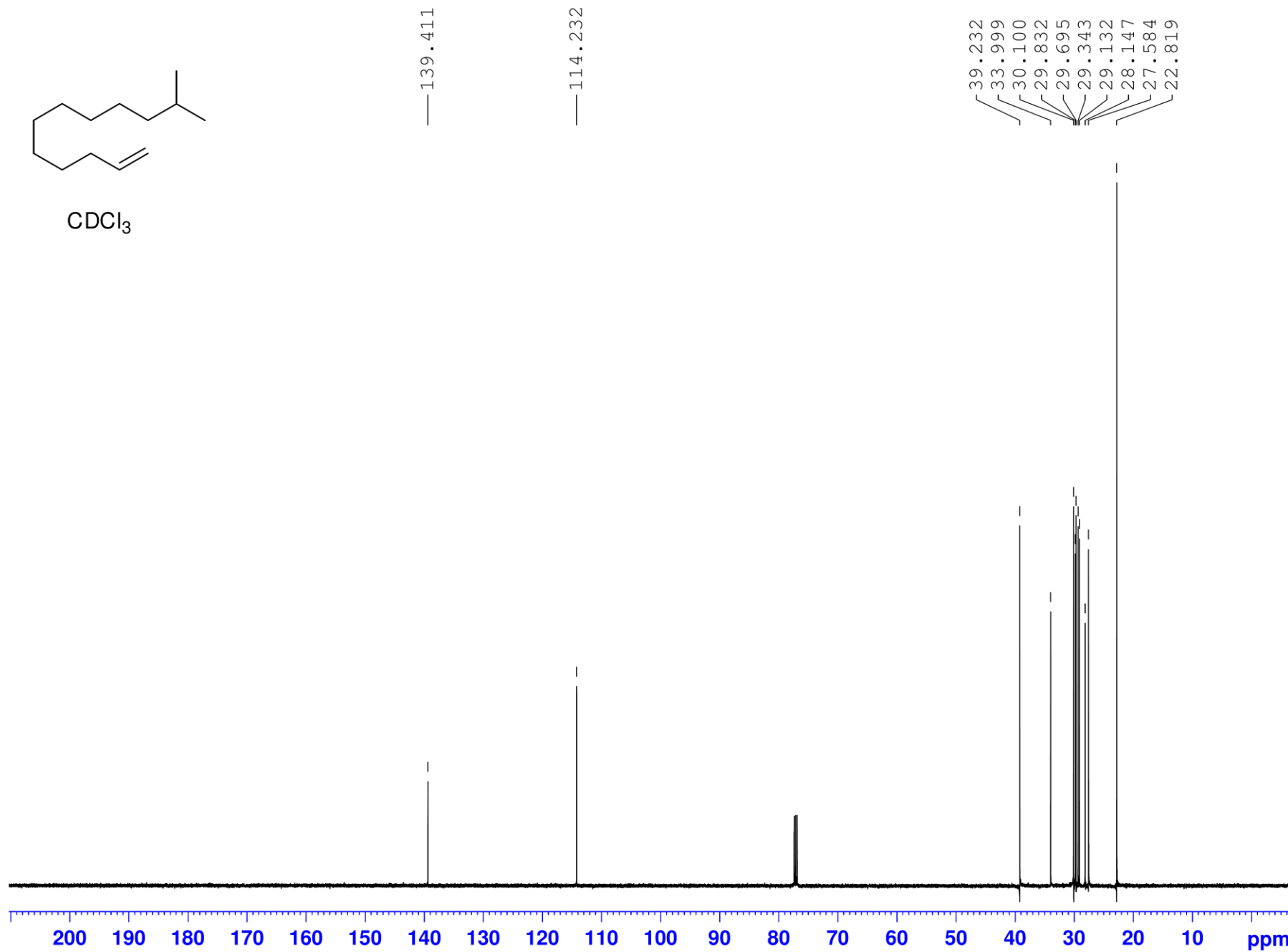
CDCl<sub>3</sub>



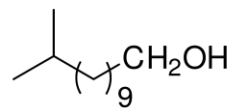
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 11-Methyldodec-1-ene (**11**)



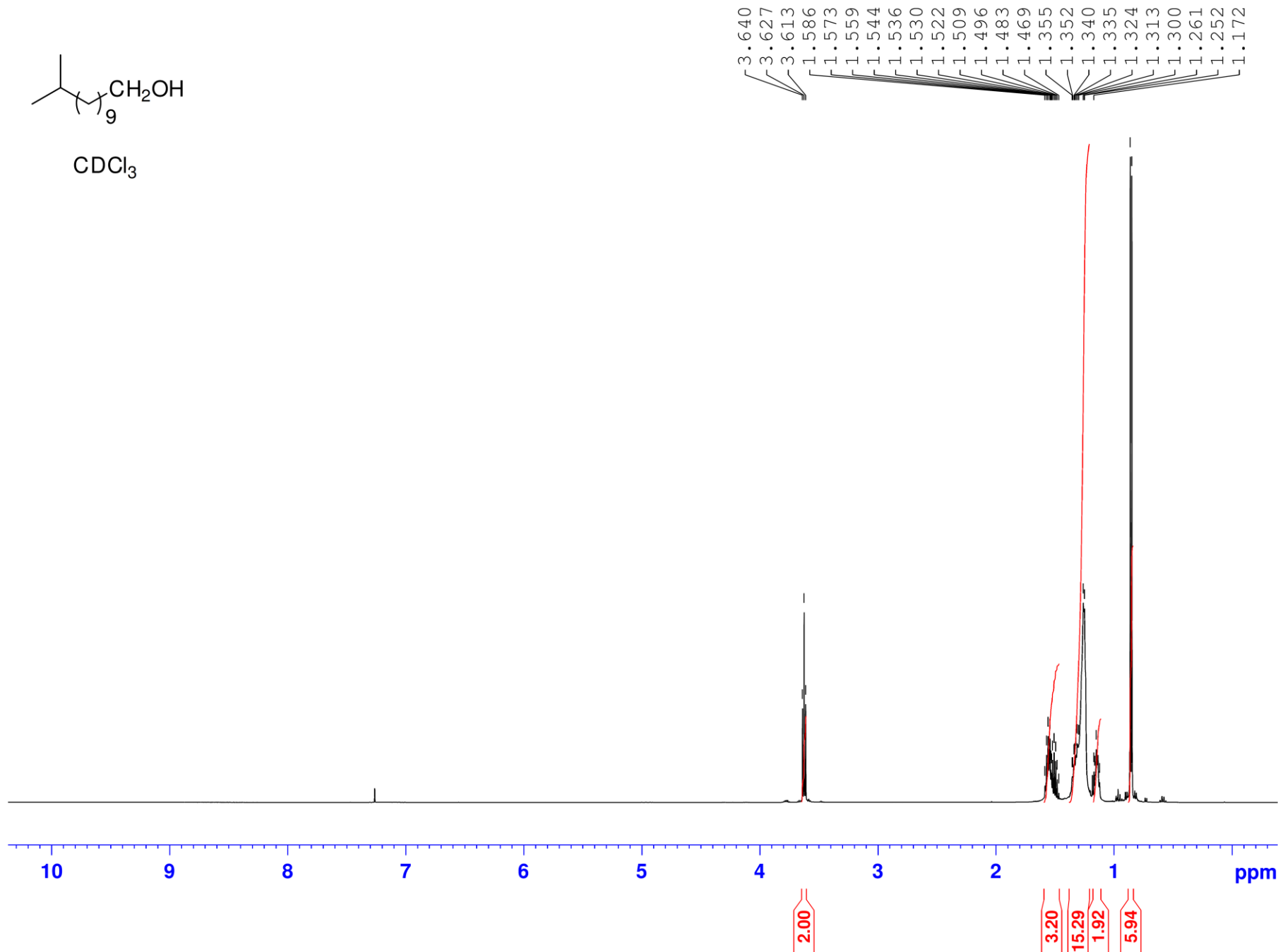
$\text{CDCl}_3$



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) – 11-Methyldodecan-1-ol (**12**)

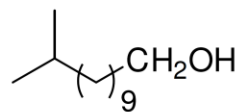


$\text{CDCl}_3$





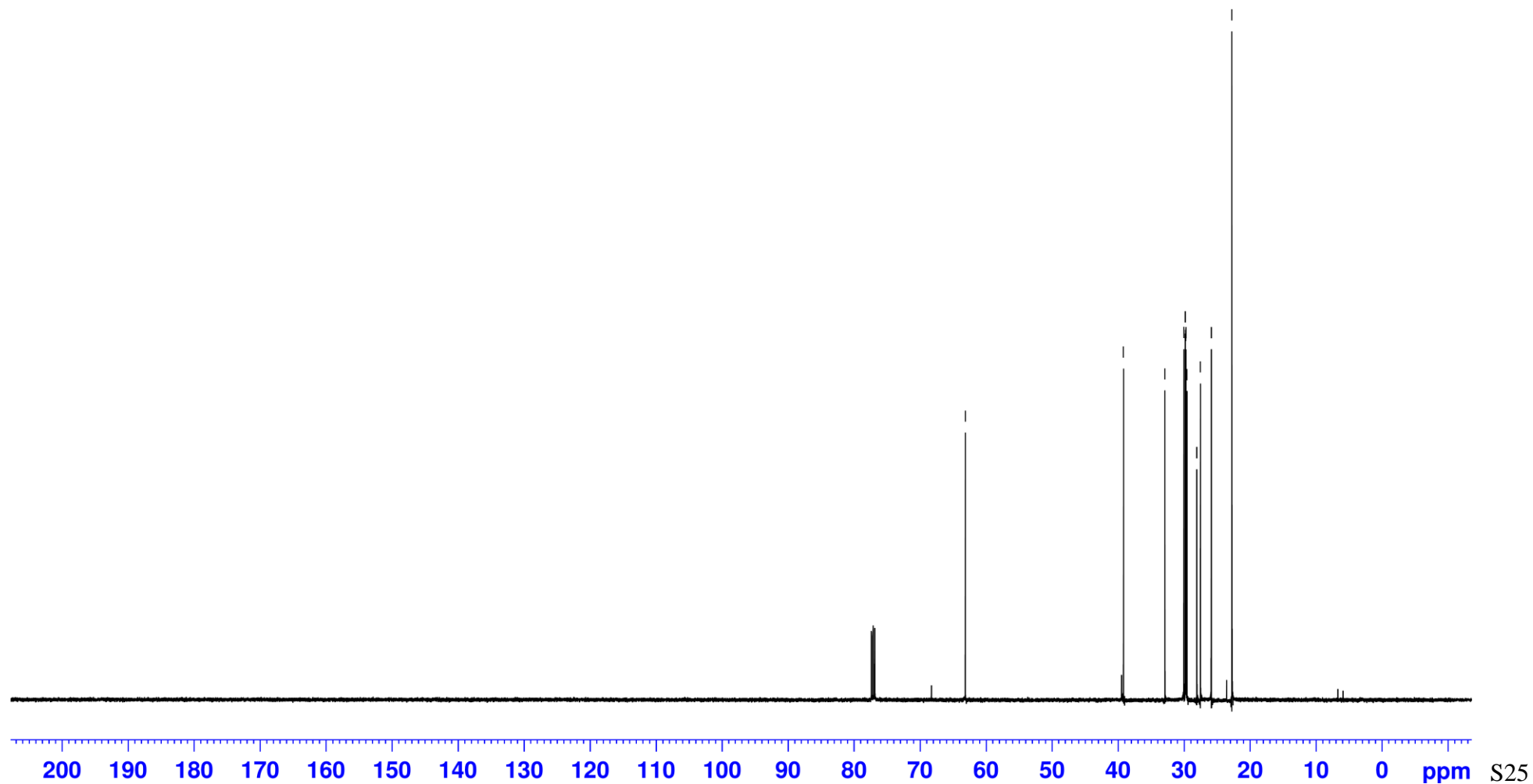
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 11-Methyldodecan-1-ol (**12**)



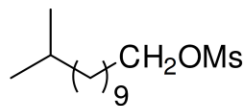
$\text{CDCl}_3$

— 63.175

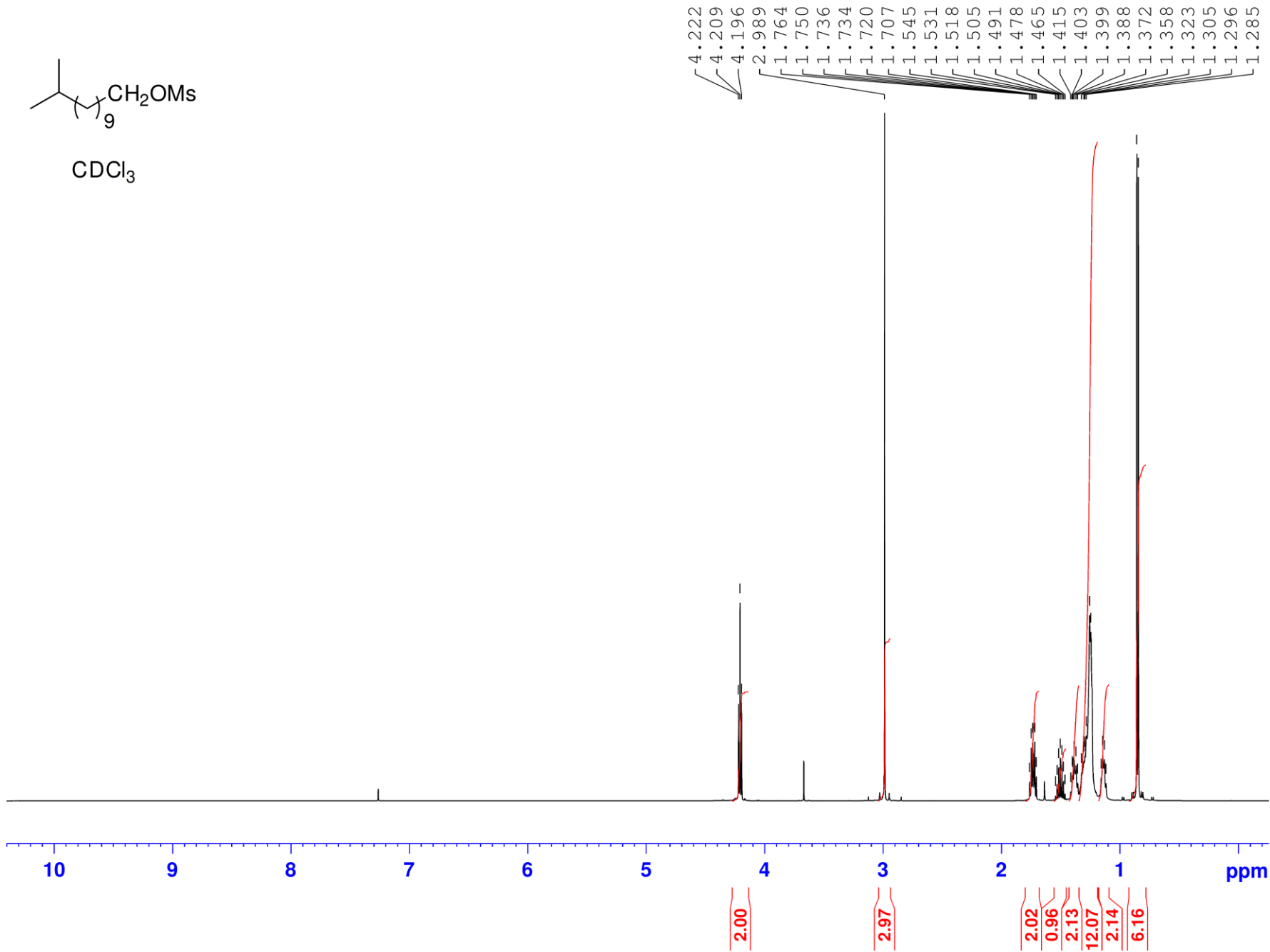
39.196  
32.941  
30.069  
29.832  
29.763  
29.746  
29.581  
28.103  
27.549  
25.889  
22.785



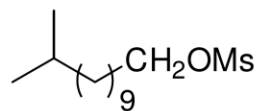
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – 11-Methyldodecyl methanesulfonate (**13**)



CDCl<sub>3</sub>



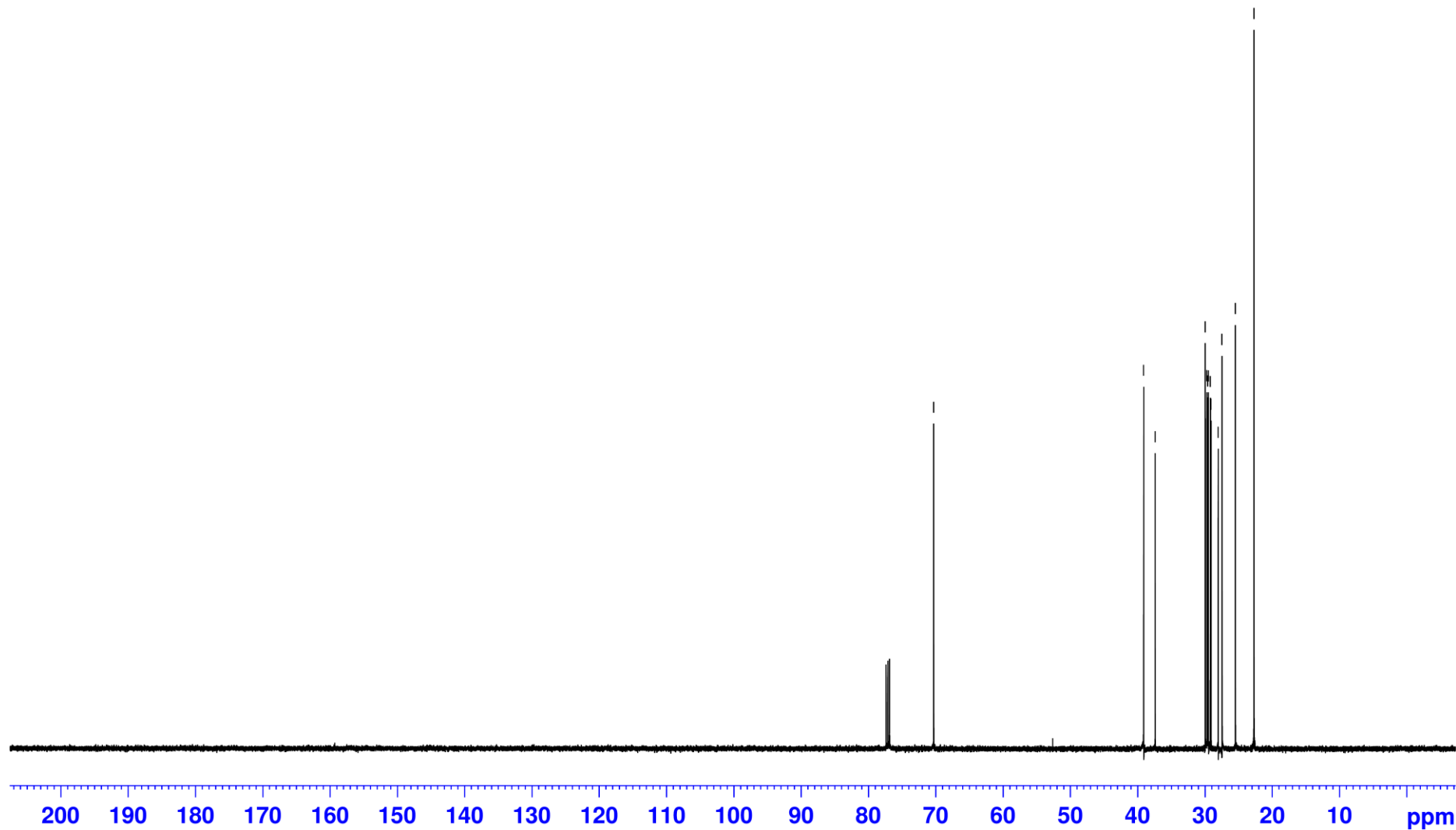
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 11-Methyldodecyl methanesulfonate (**13**)



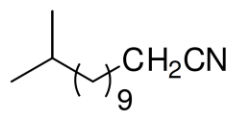
$\text{CDCl}_3$

— 70.336

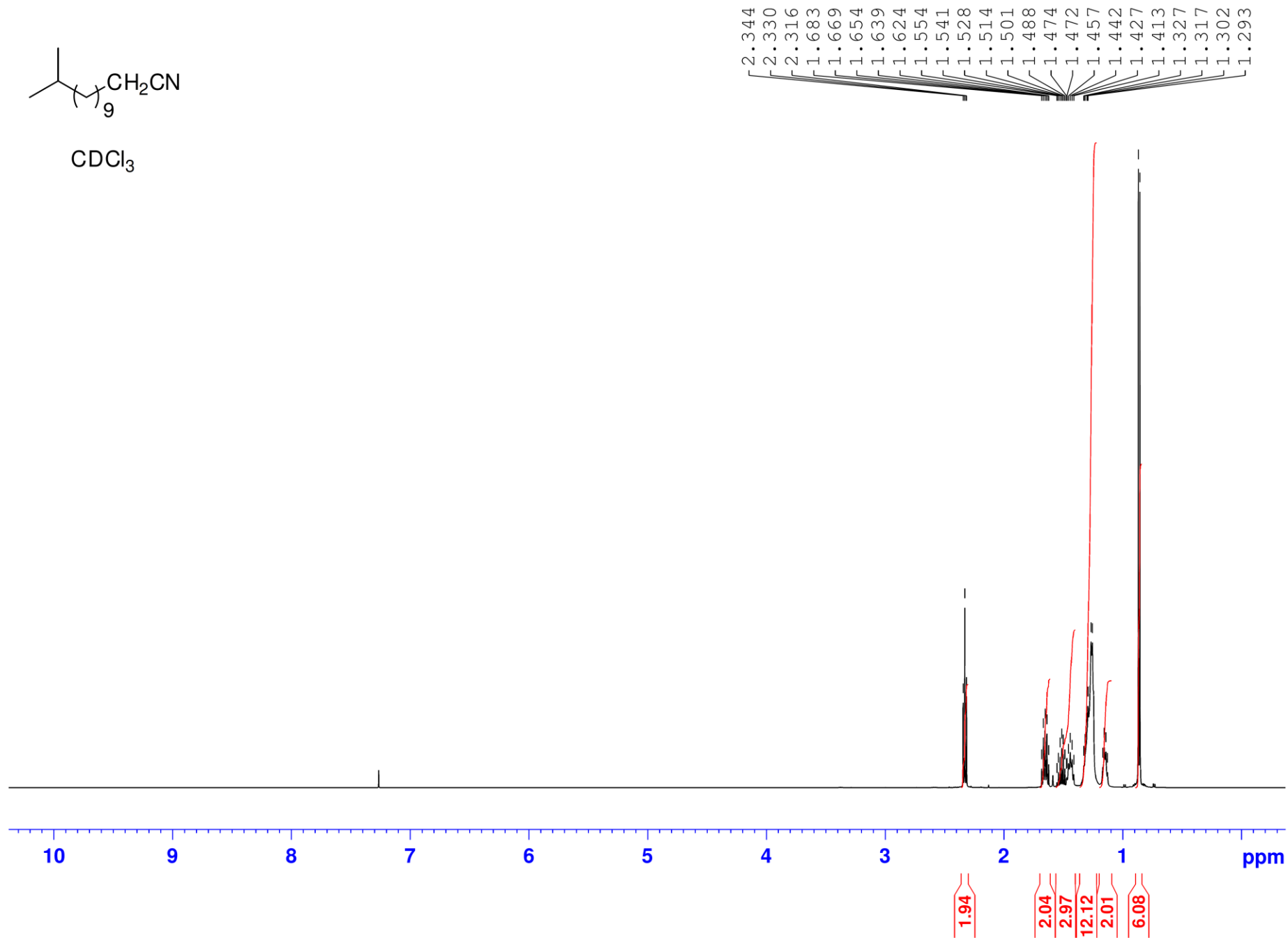
39.138  
37.428  
29.990  
29.730  
29.614  
29.519  
29.224  
29.125  
28.055  
27.488  
25.515  
22.750



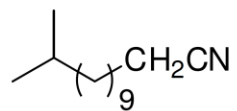
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) – 12-Methyltridecanenitrile (**14**)



$\text{CDCl}_3$



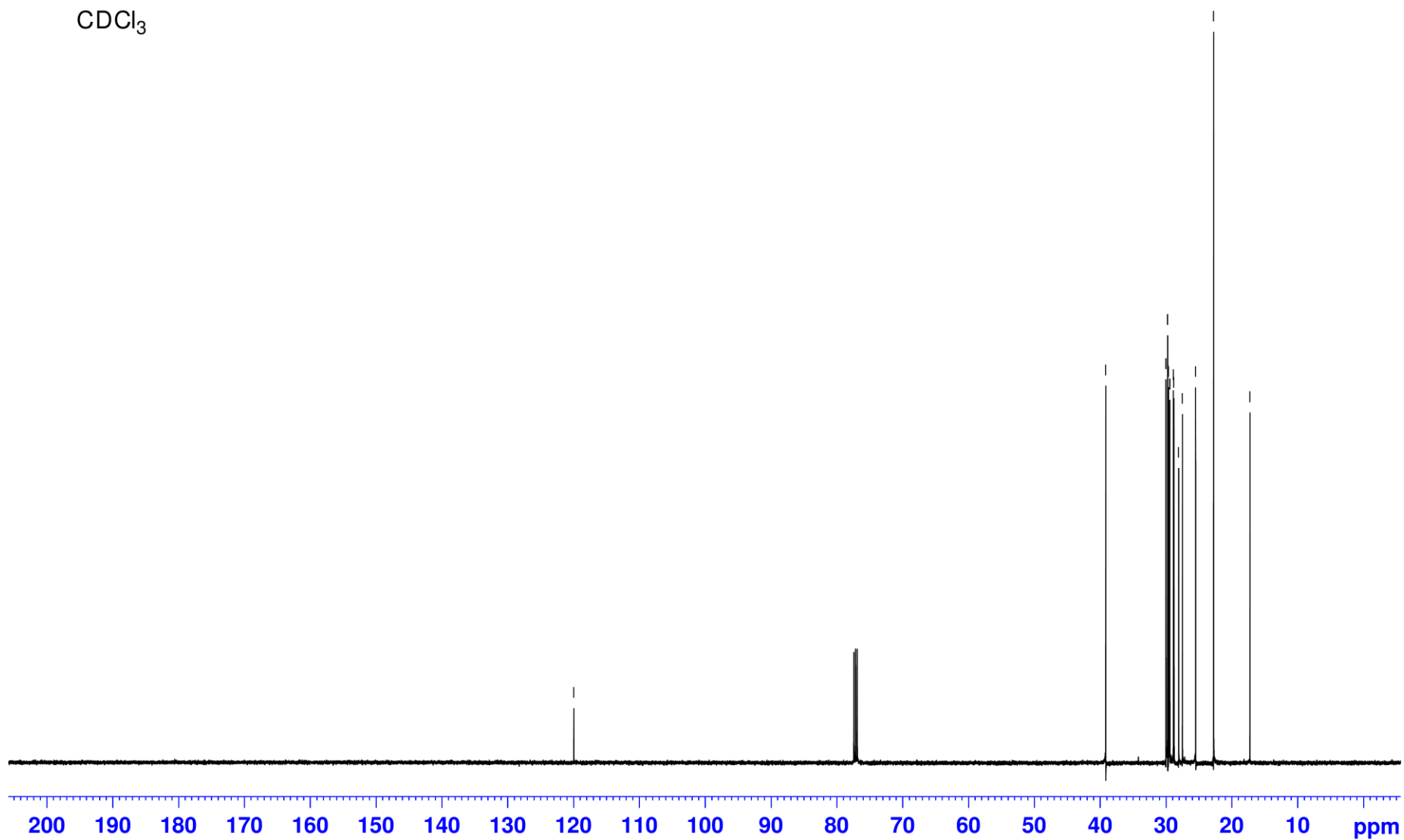
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 12-Methyltridecanenitrile (**14**)



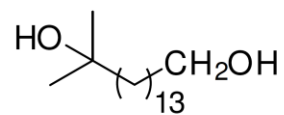
$\text{CDCl}_3$

— 119.971

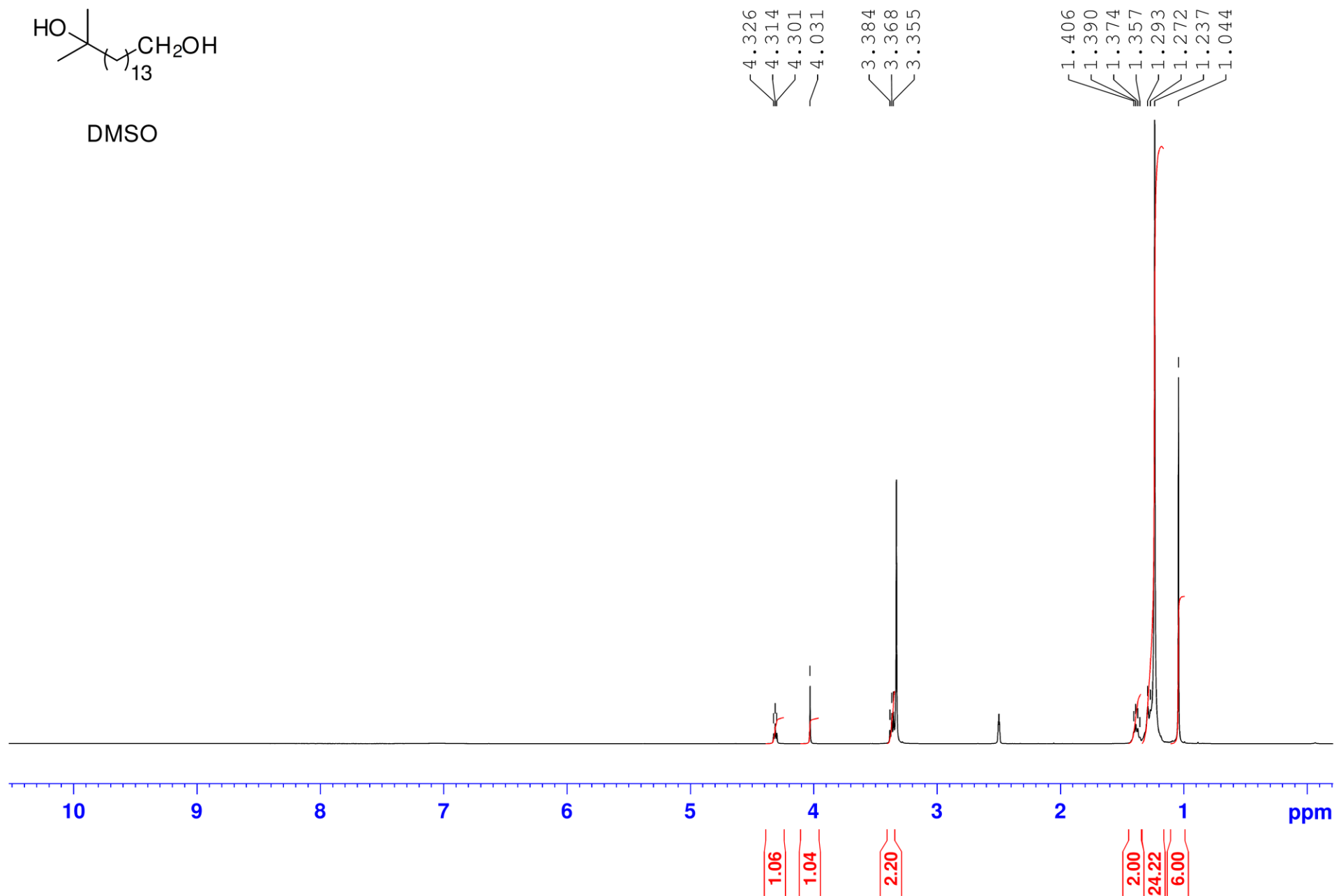
39.166  
30.011  
29.744  
29.626  
29.430  
28.888  
28.793  
28.088  
27.514  
25.507  
22.776  
17.246



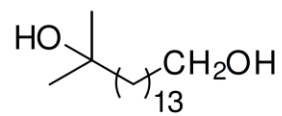
<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) – 15-Methylhexadecane-1,15-diol (**16**)



DMSO

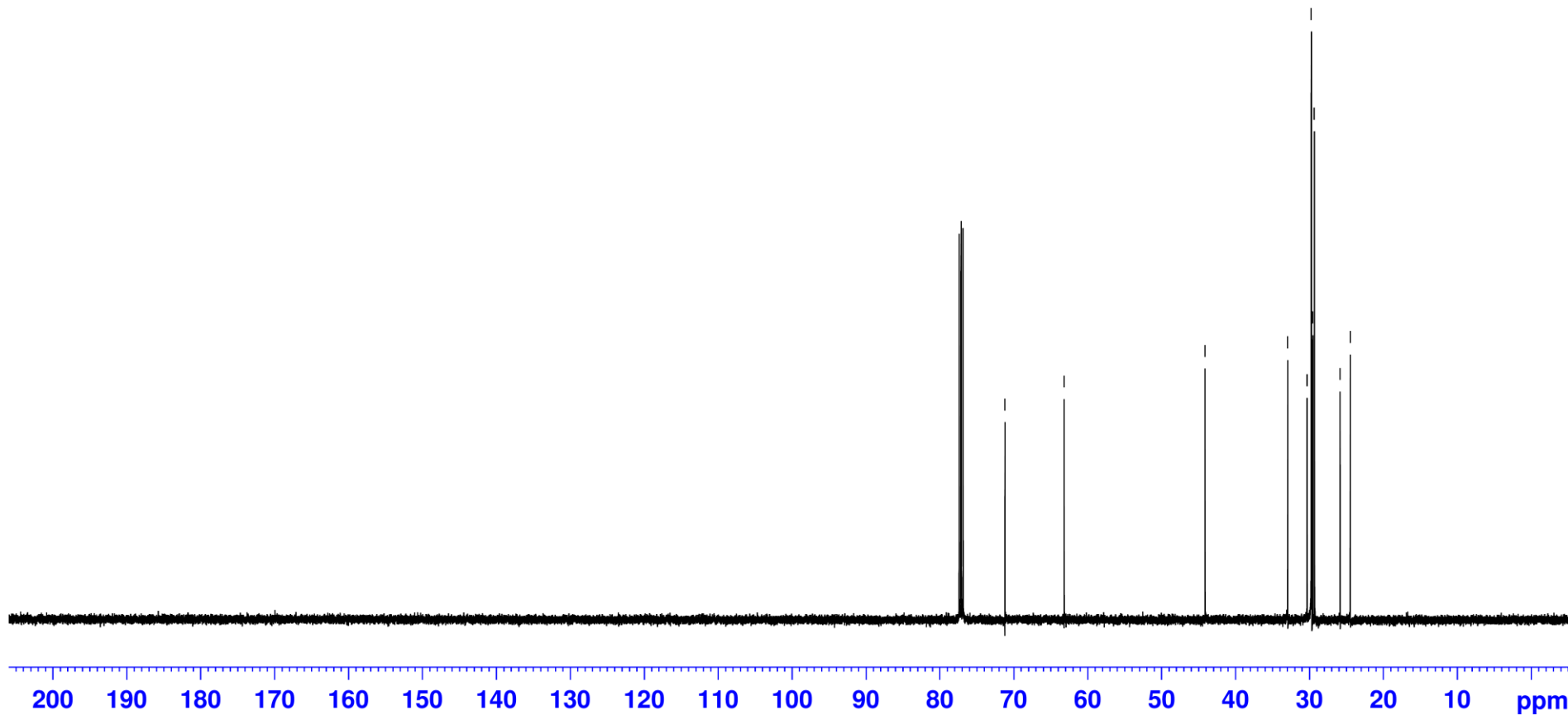


$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 15-Methylhexadecane-1,15-diol (**16**)

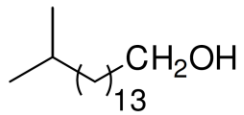


$\text{CDCl}_3$

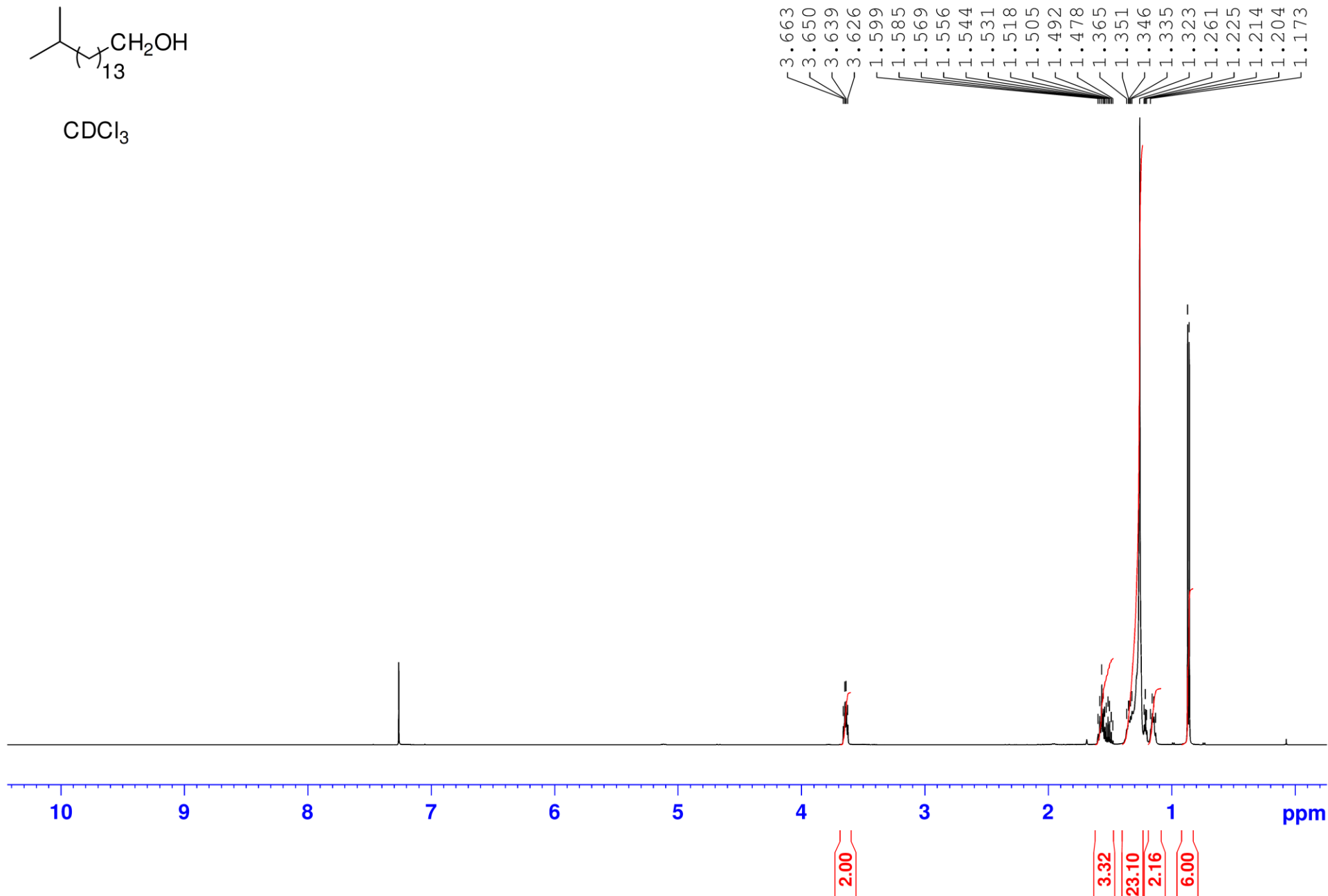
— 71.223  
— 63.225  
44.149  
32.959  
30.338  
29.785  
29.748  
29.743  
29.721  
29.571  
29.360  
25.883  
24.503



<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – 15-Methylhexadecan-1-ol (**17**)

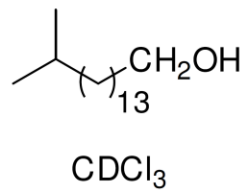


CDCl<sub>3</sub>

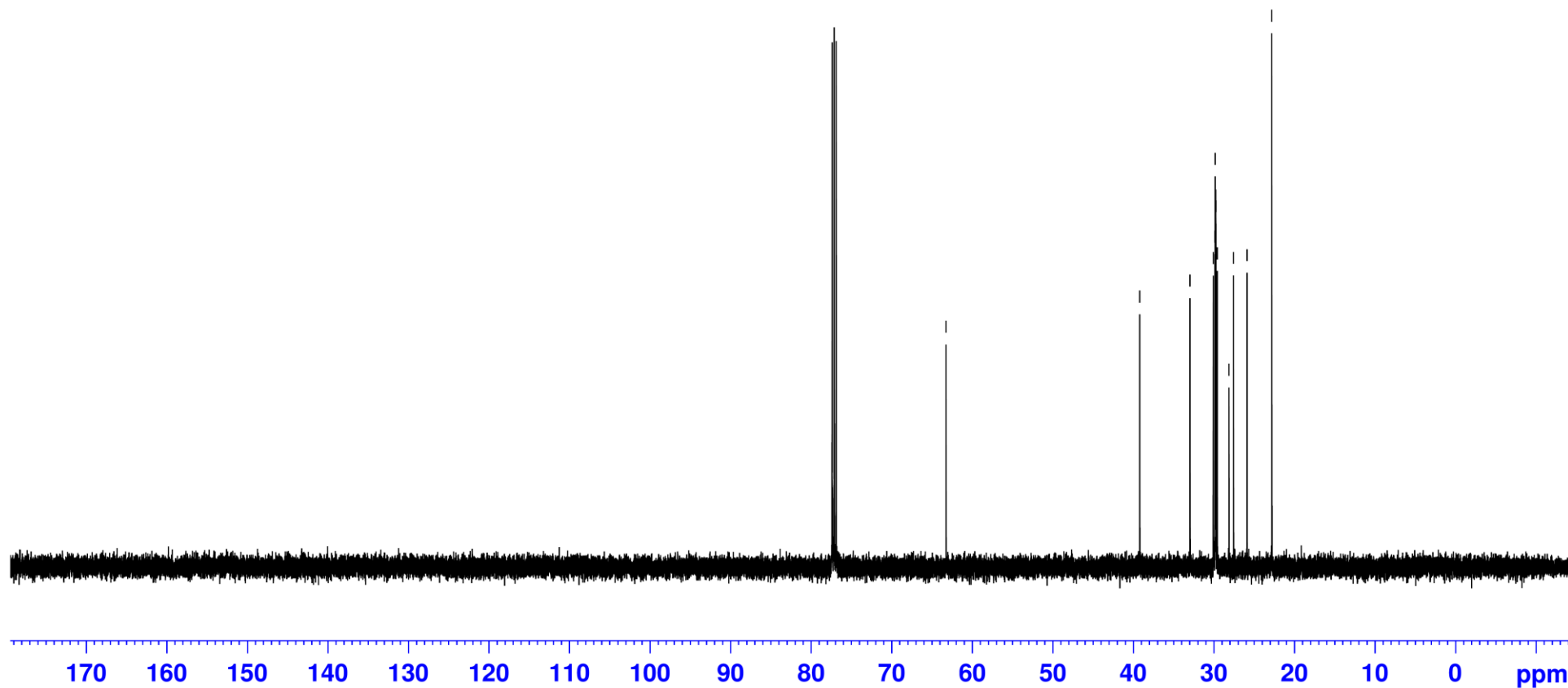




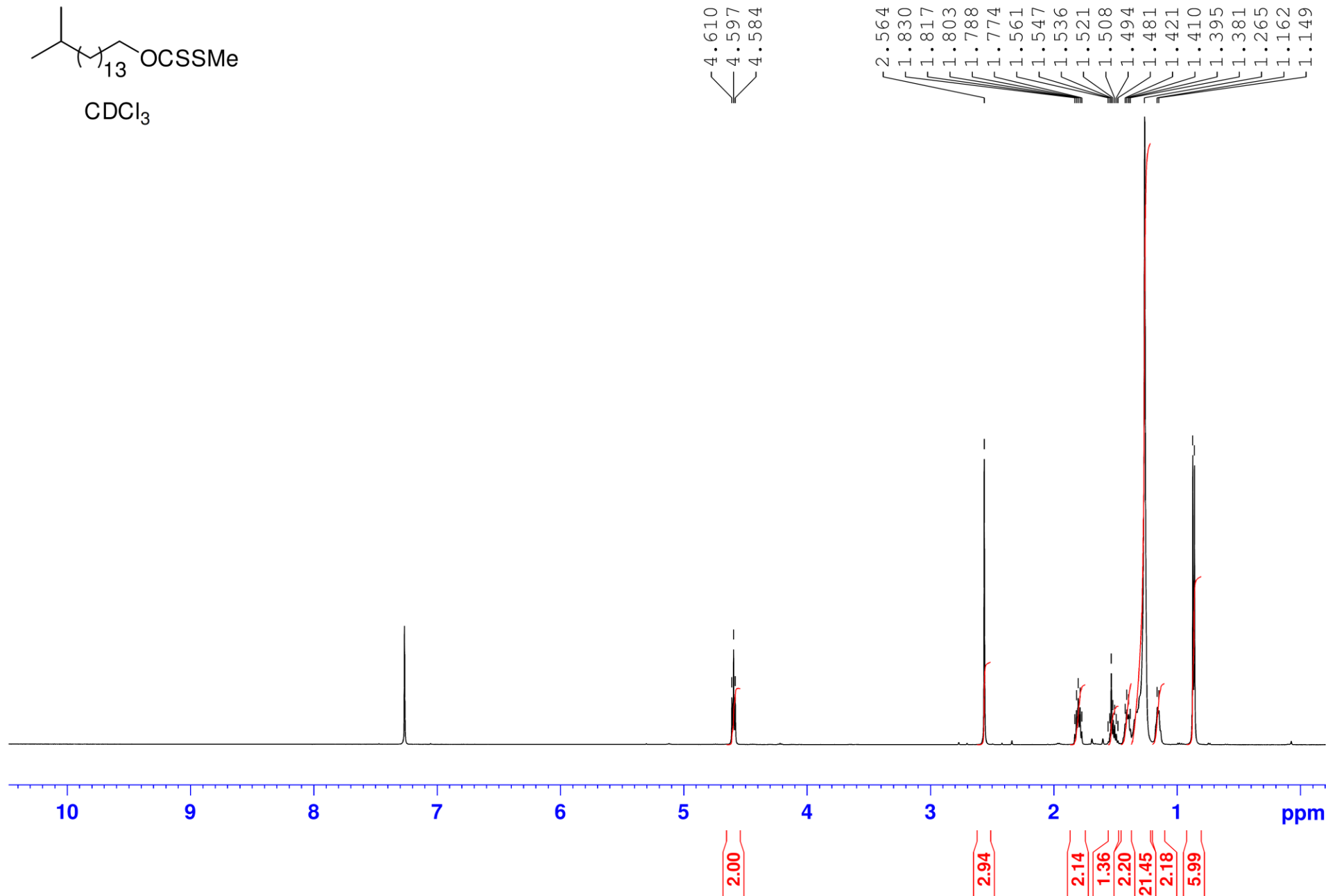
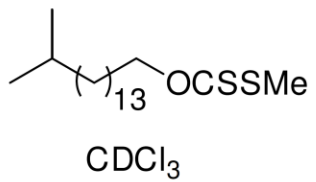
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 15-Methylhexadecan-1-ol (**17**)



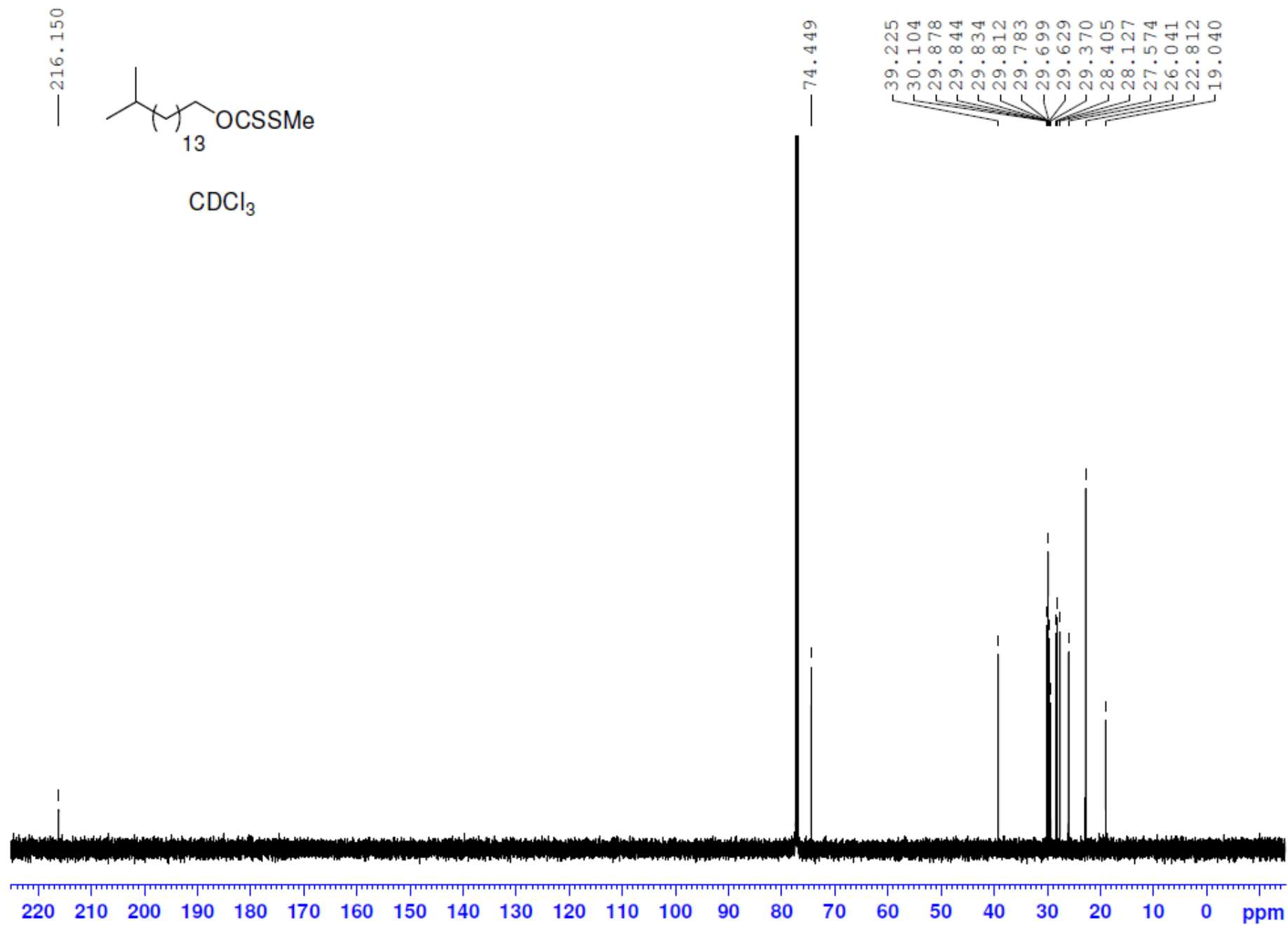
— 63.270  
39.220  
32.980  
30.103  
29.881  
29.849  
29.845  
29.829  
29.814  
29.771  
29.754  
29.592  
28.127  
27.576  
25.895  
22.816



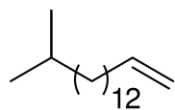
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – *S*-Methyl-*O*-15-methylhexadecyl dithiocarbonate (**18**)



$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – *S*-Methyl-*O*-15-methylhexadecyl dithiocarbonate (**18**)

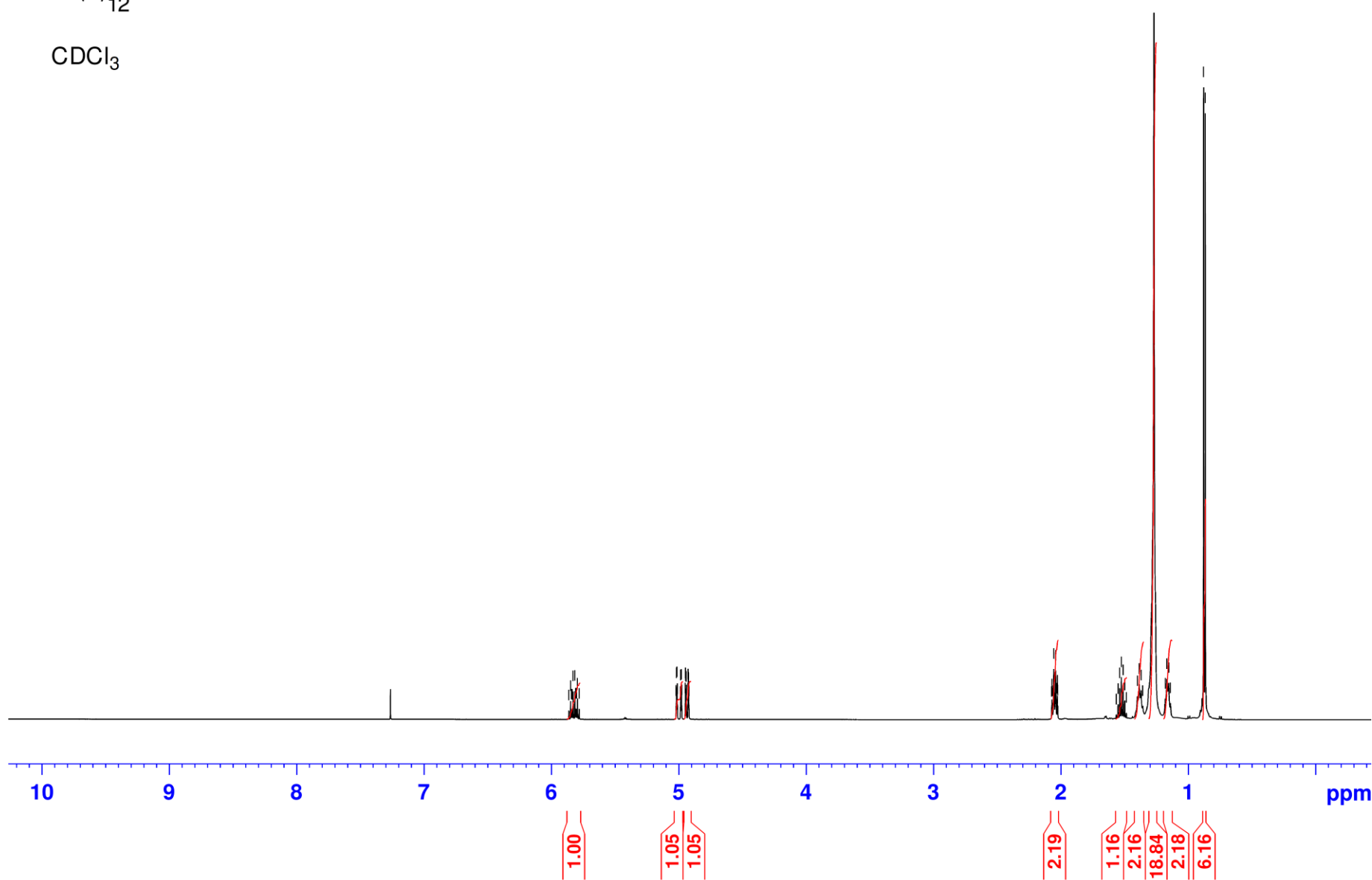


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – 15-Methylhexadecan-1-ene (**19**)

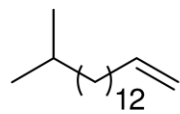


CDCl<sub>3</sub>

5.864  
5.850  
5.843  
5.837  
5.830  
5.816  
5.809  
5.803  
5.796  
5.782  
5.023  
5.019  
5.015  
5.012  
4.988  
4.985  
4.981  
4.978  
4.950  
4.947  
4.945  
4.943  
4.941  
4.930  
4.927  
4.925  
4.923  
4.920  
2.073  
2.071  
2.068  
2.057  
2.043  
2.041  
2.031  
2.028  
2.025  
1.565  
1.552  
1.539  
1.526  
1.512  
1.499  
1.486  
1.400  
1.386  
1.371  
1.358



<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) – 15-Methylhexadecan-1-ene (**19**)

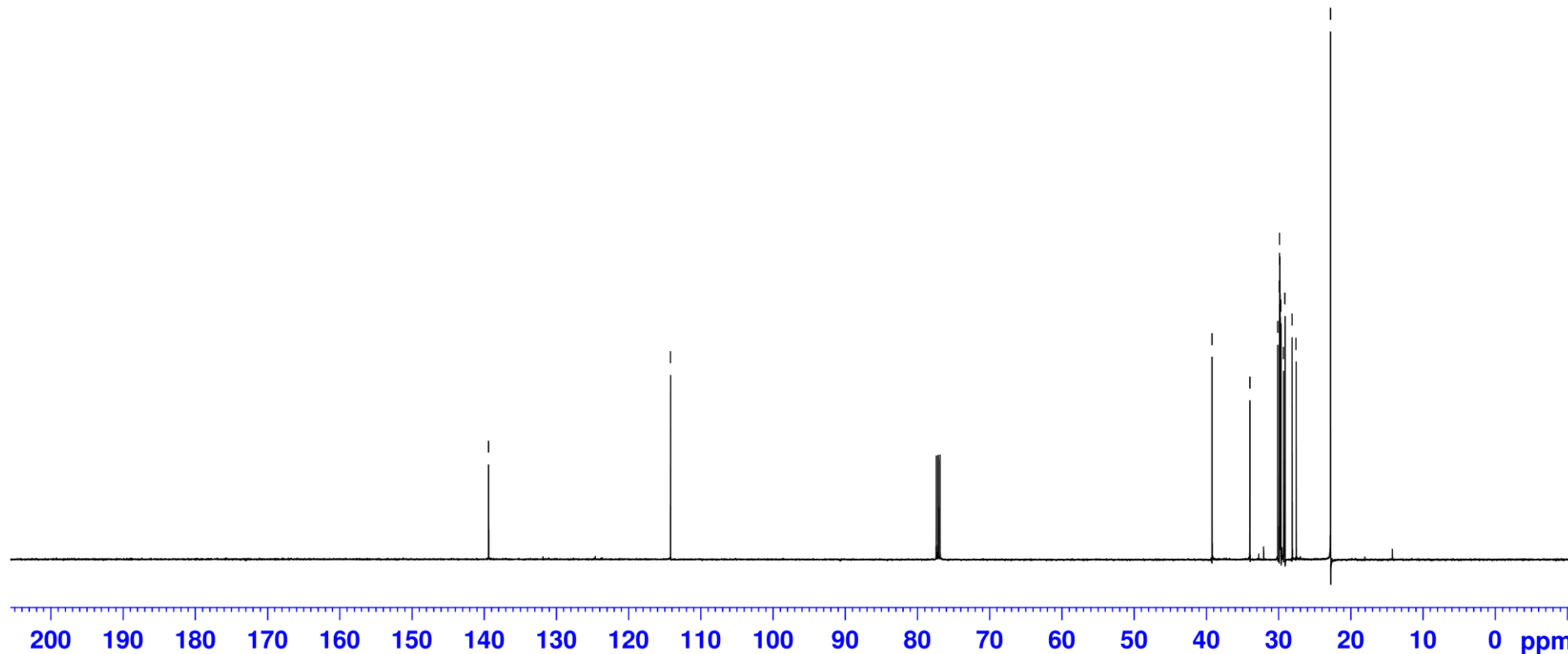


CDCl<sub>3</sub>

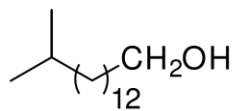
— 139.418

— 114.225

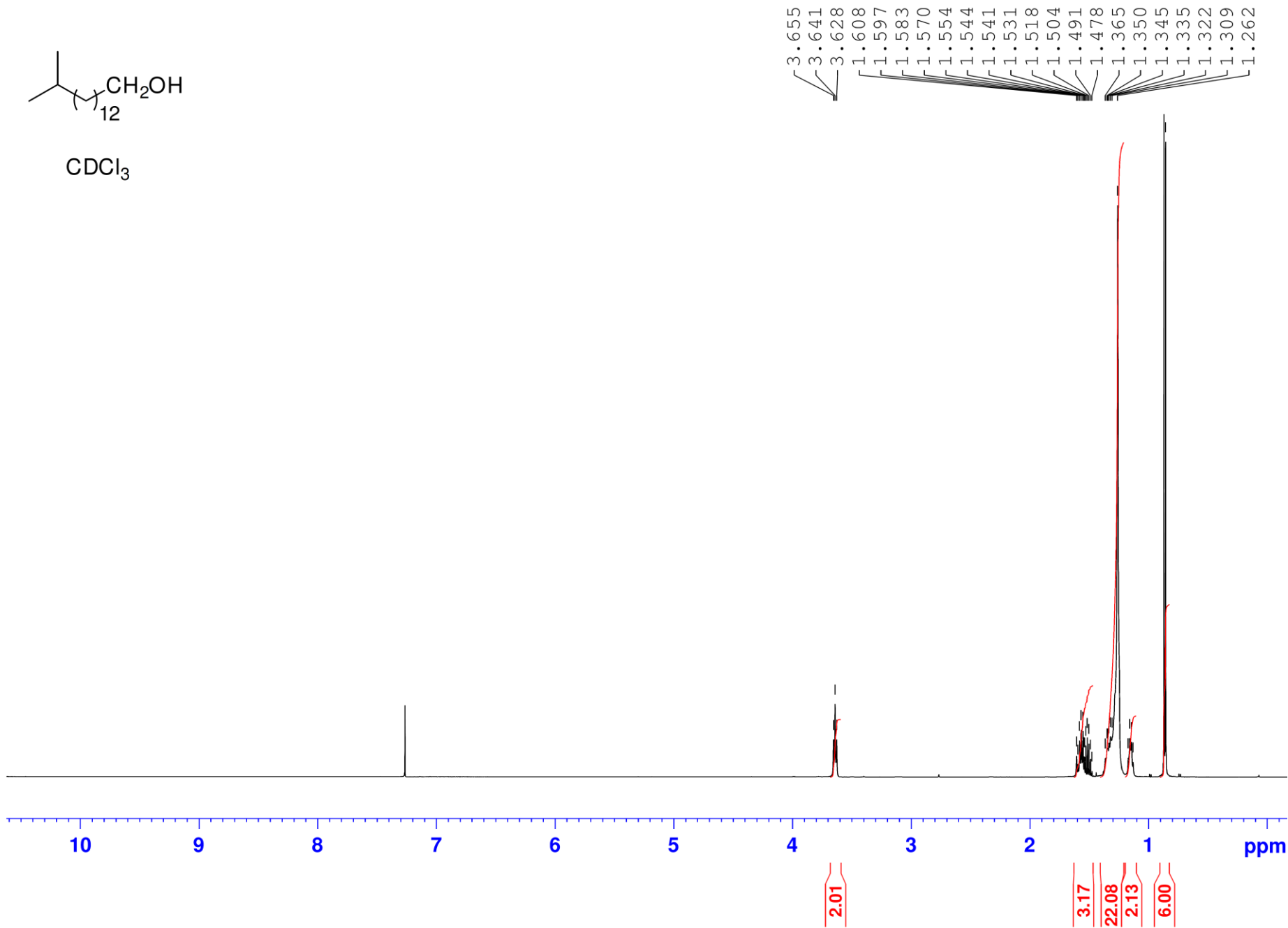
39.246  
33.993  
30.125  
29.900  
29.863  
29.857  
29.839  
29.794  
29.687  
29.335  
29.135  
28.146  
27.596  
22.821



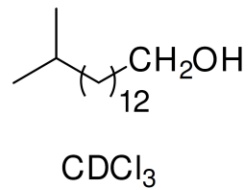
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) – 14-Methylpentadecan-1-ol (**20**)



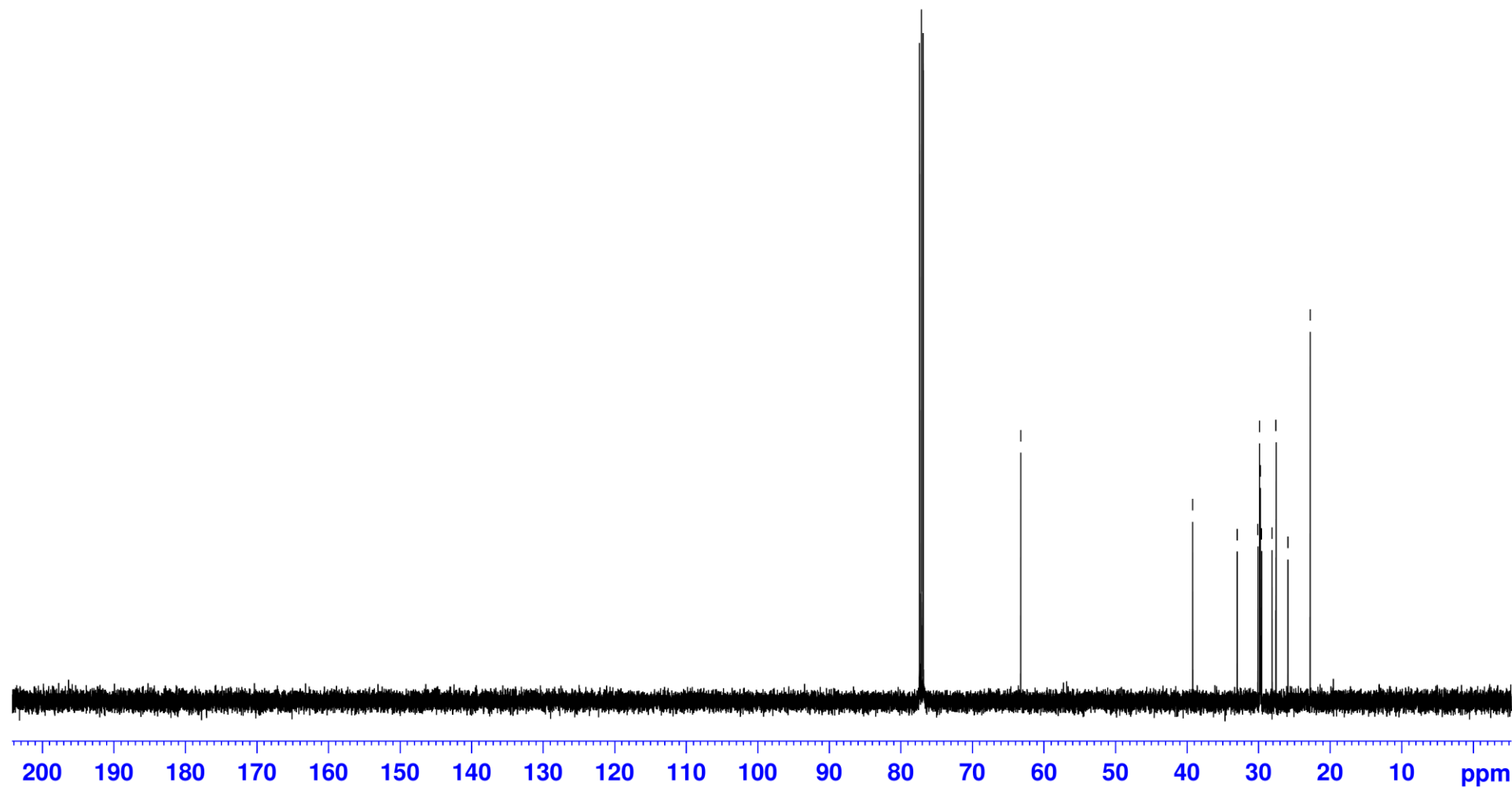
$\text{CDCl}_3$



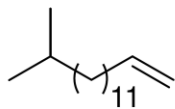
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 14-Methylpentadecan-1-ol (**20**)



63.257  
39.224  
32.983  
30.101  
29.874  
29.840  
29.830  
29.809  
29.767  
29.753  
29.592  
28.125  
27.571  
25.900  
22.806

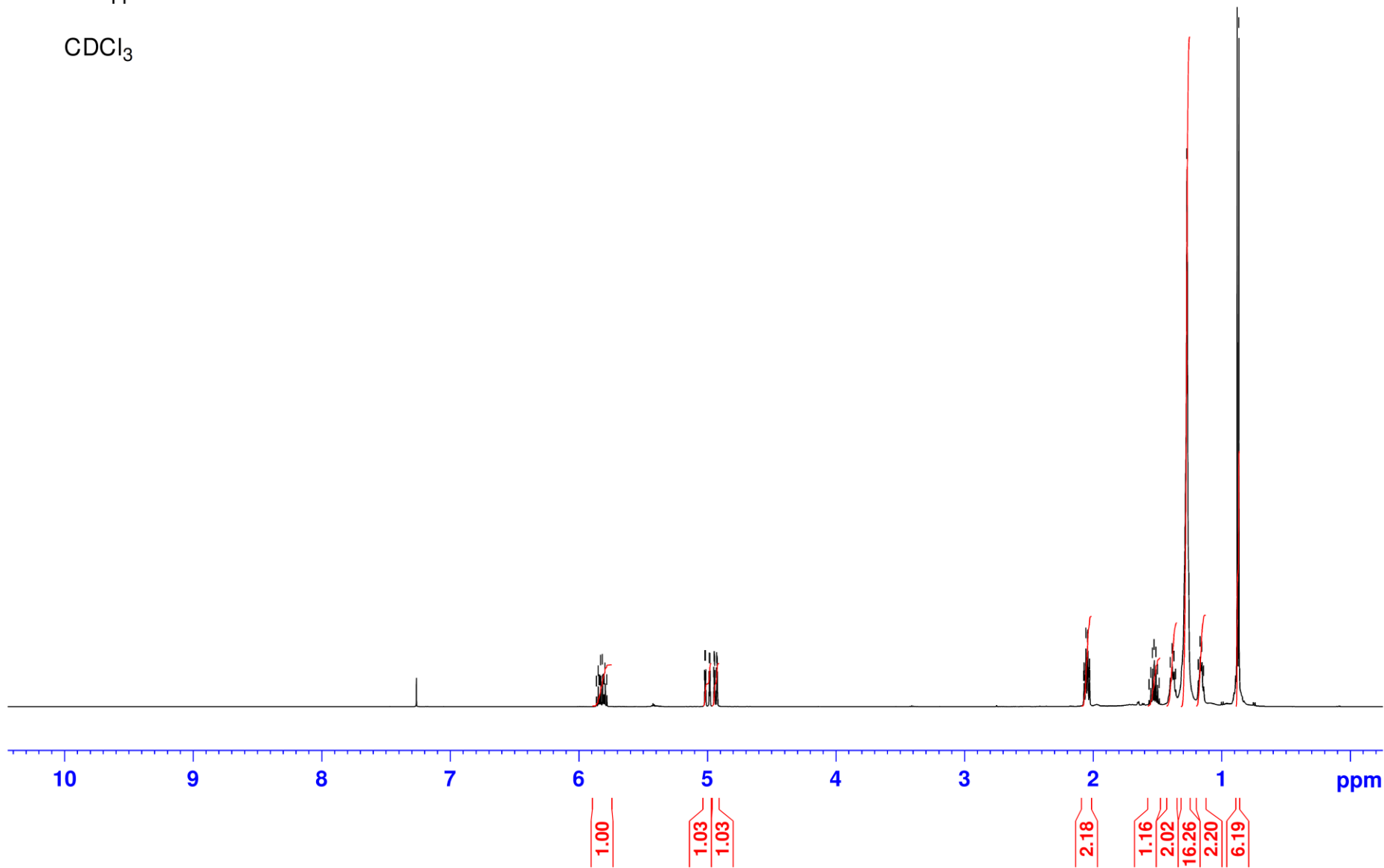


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – 14-Methylpentadec-1-ene (**22**)



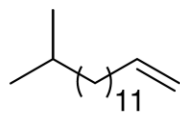
CDCl<sub>3</sub>

5.864  
5.851  
5.844  
5.838  
5.830  
5.817  
5.810  
5.803  
5.796  
5.783  
5.024  
5.020  
5.016  
5.013  
4.989  
4.986  
4.982  
4.979  
4.951  
4.948  
4.946  
4.944  
4.942  
4.930  
4.928  
4.926  
4.924  
4.922  
2.074  
2.072  
2.069  
2.058  
2.044  
2.043  
2.031  
2.029  
2.026  
1.566  
1.553  
1.540  
1.526  
1.513  
1.500  
1.486  
1.401  
1.387  
1.372





$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 14-Methylpentadec-1-ene (**22**)

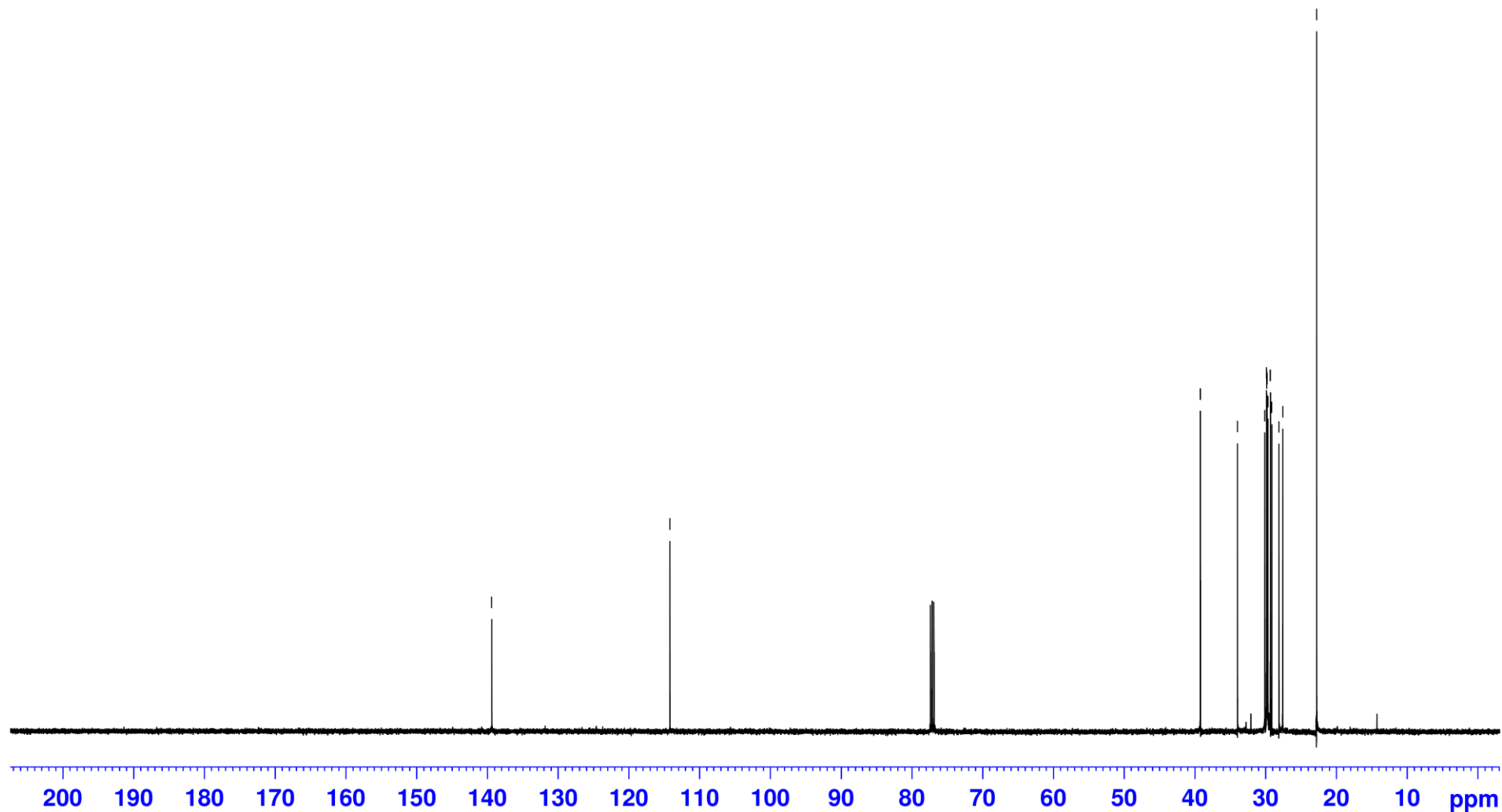


$\text{CDCl}_3$

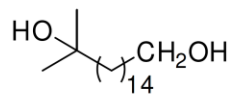
— 139.413

— 114.229

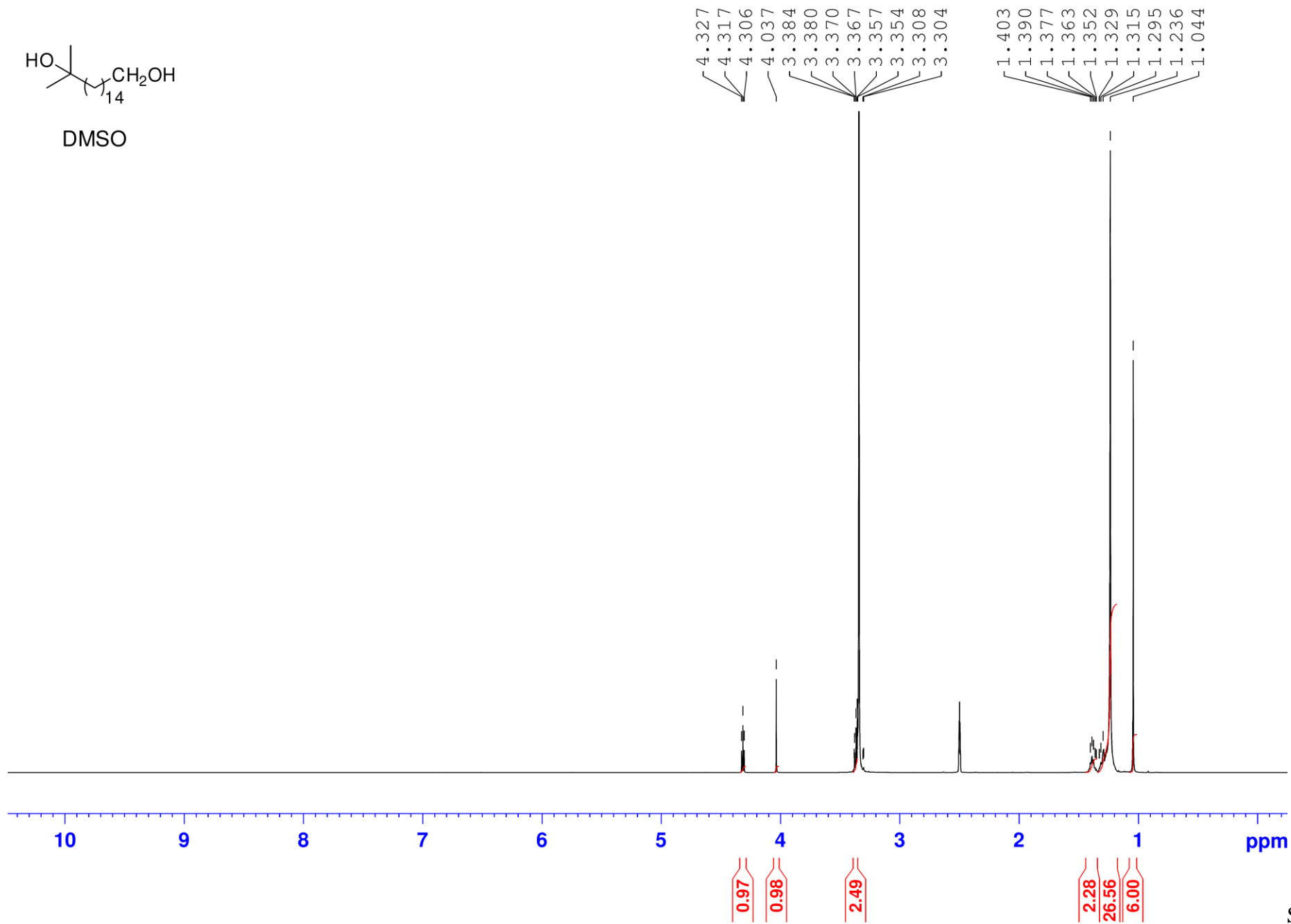
39.245  
34.001  
30.130  
29.902  
29.865  
29.852  
29.801  
29.694  
29.341  
29.136  
28.147  
27.603  
22.824



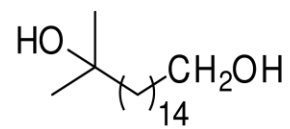
<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) – 16-Methylheptadecane-1,16-diol (**24**)



DMSO



$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 16-Methylheptadecane-1,16-diol (**24**)

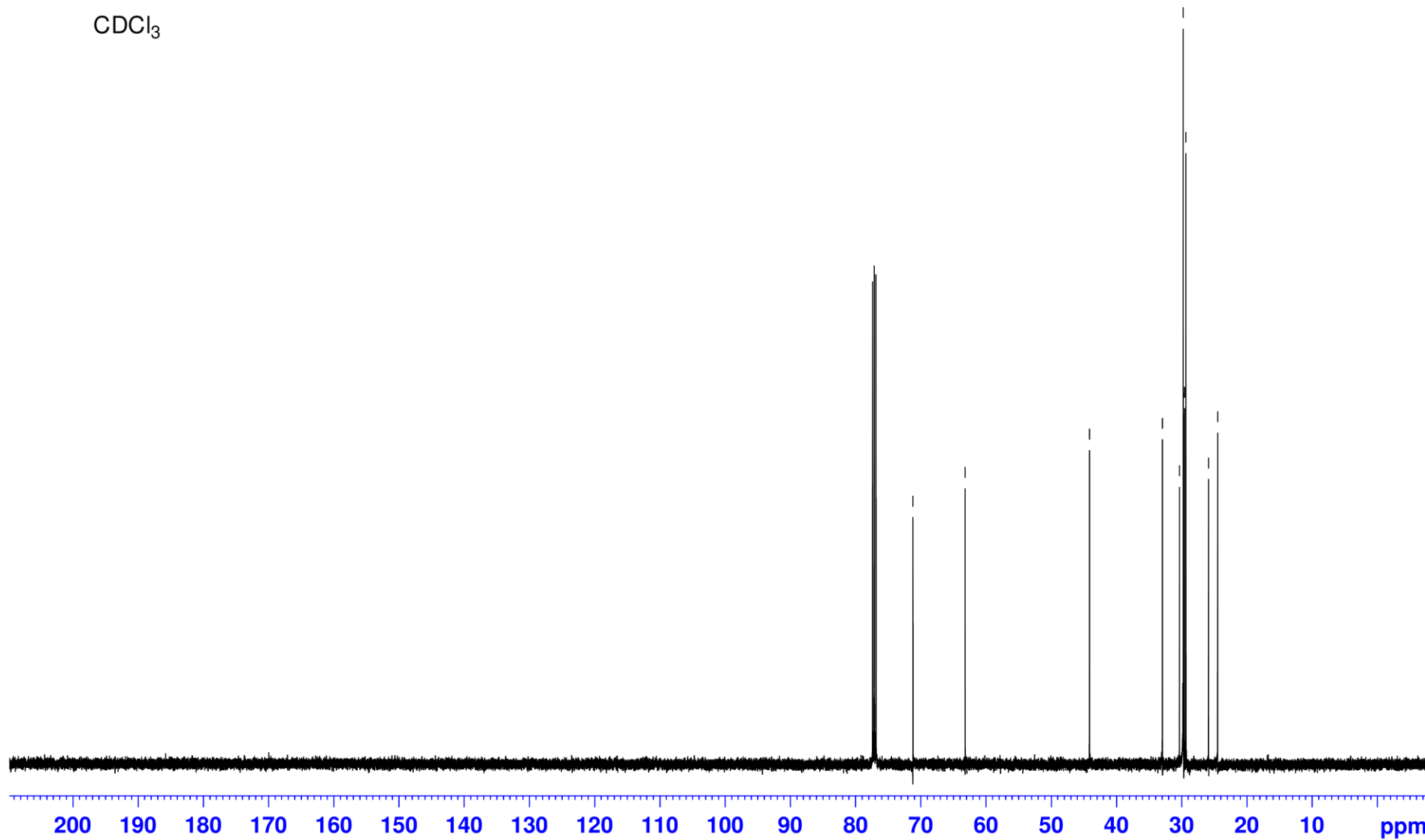


$\text{CDCl}_3$

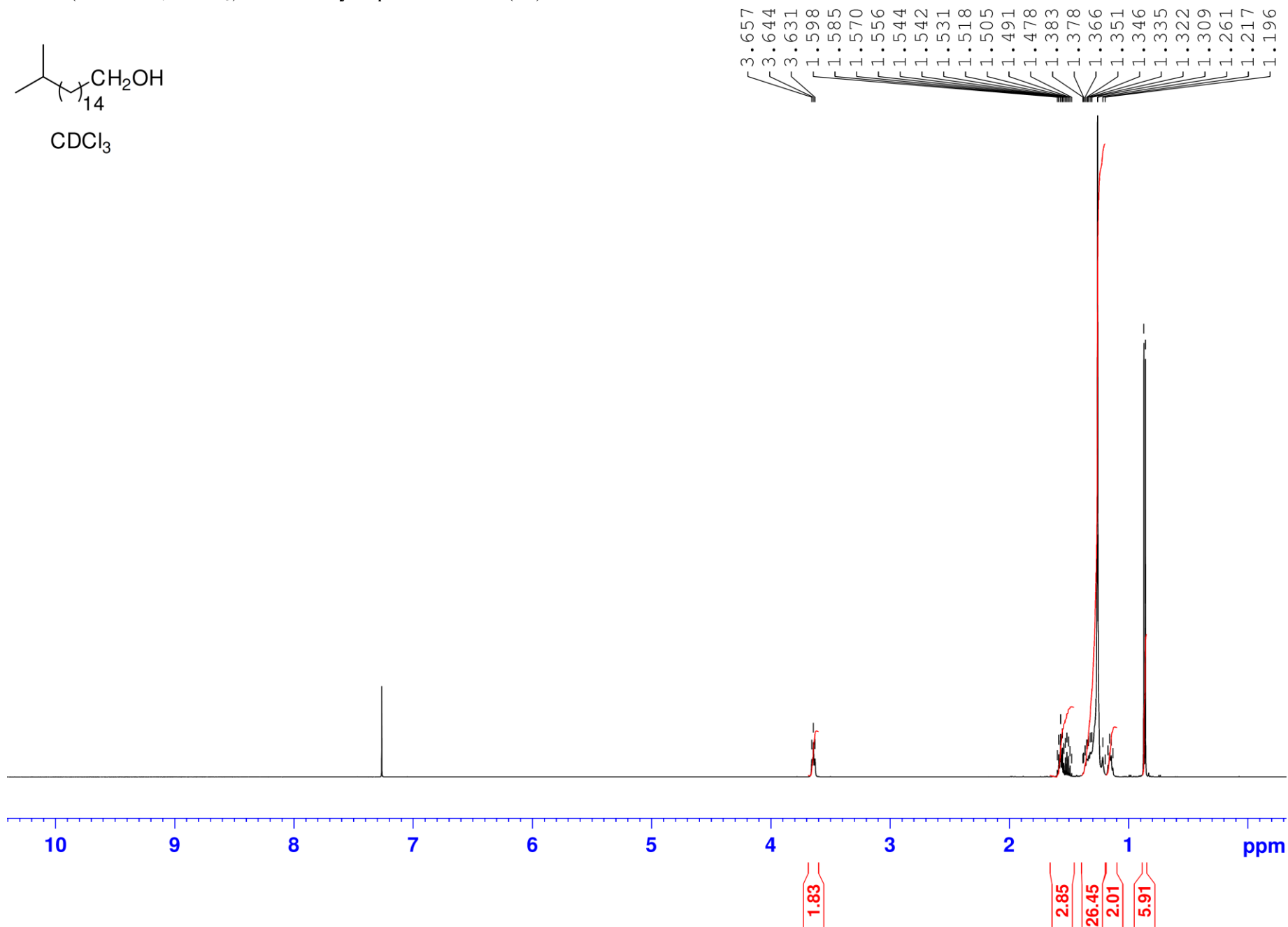
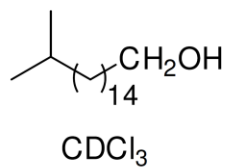
— 71.223

— 63.226

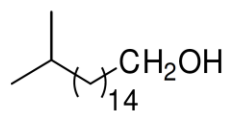
44.150  
32.959  
30.338  
29.785  
29.748  
29.743  
29.721  
29.571  
29.360  
25.884  
24.503



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) – 16-Methylheptadecan-1-ol (**25**)

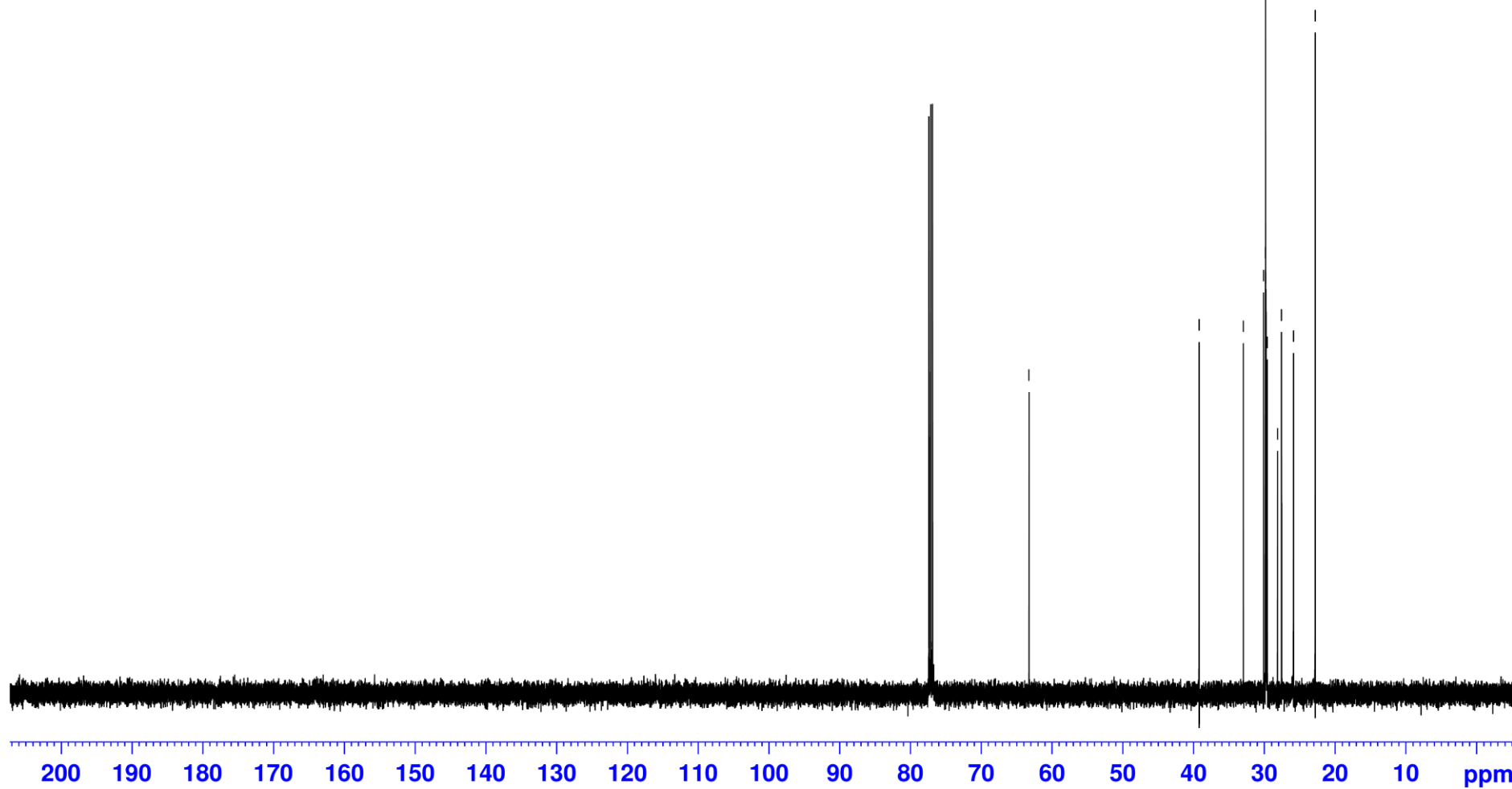


$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 16-Methylheptadecan-1-ol (**25**)

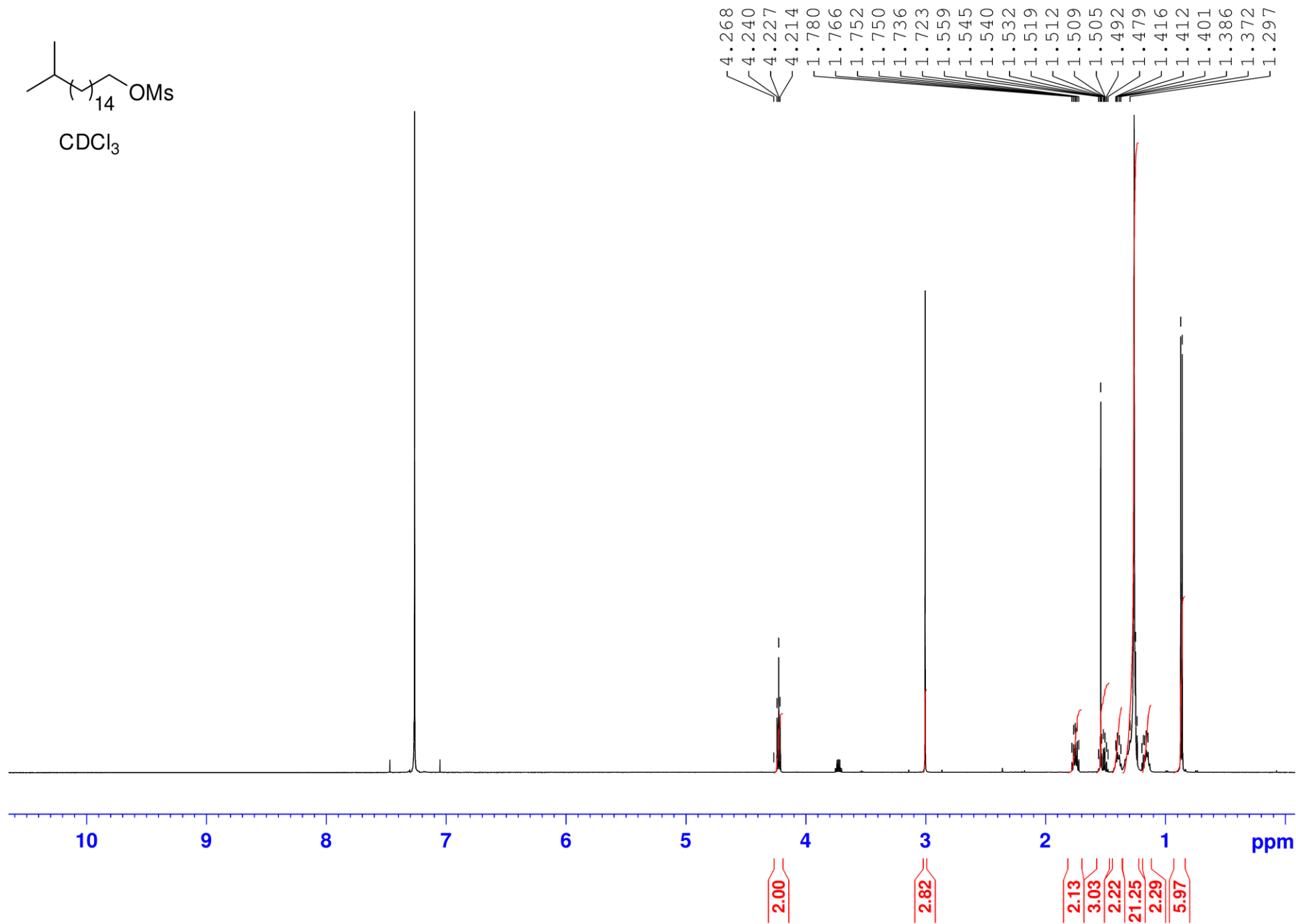
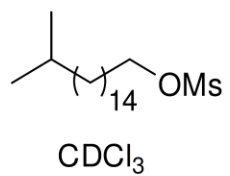


$\text{CDCl}_3$

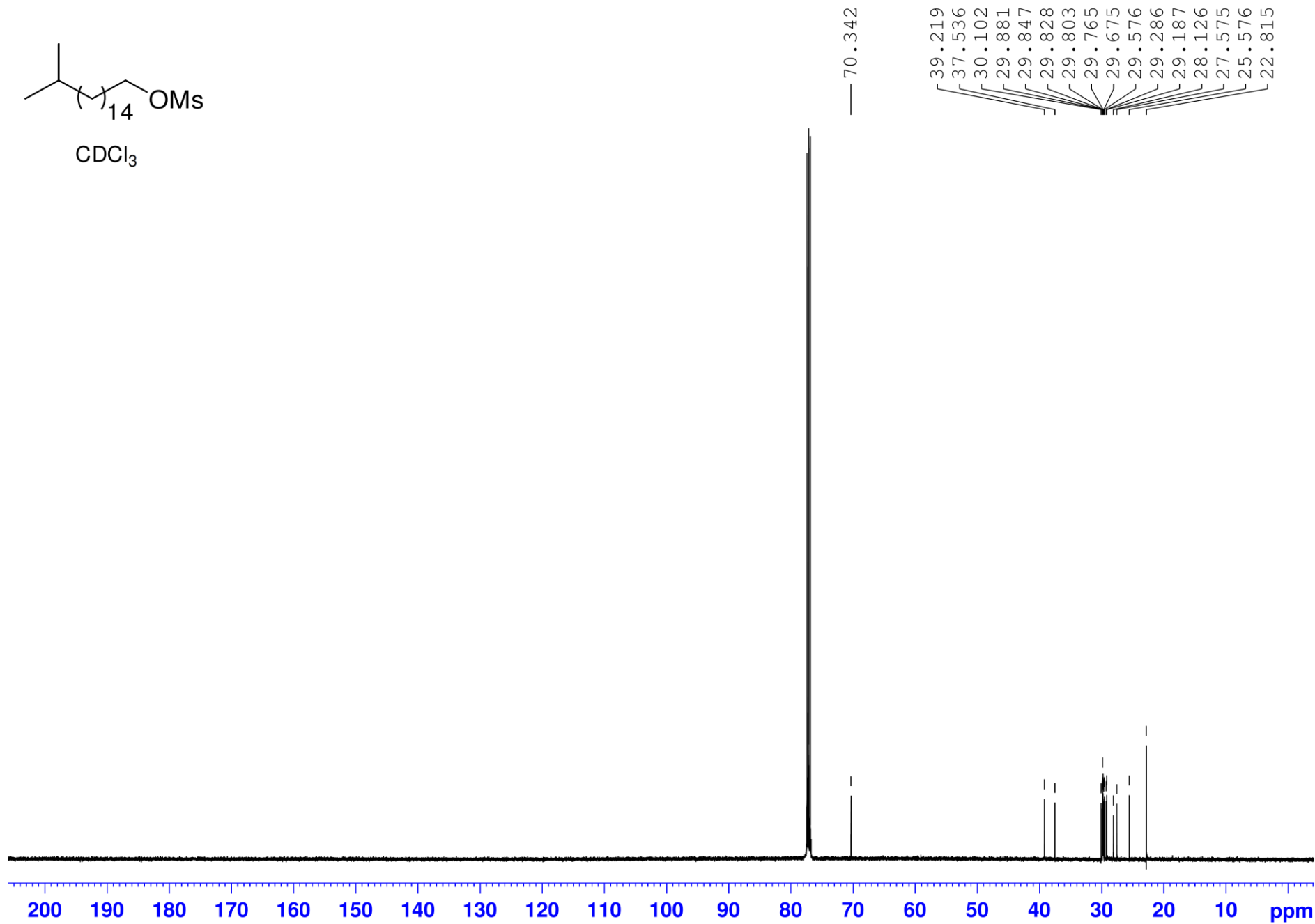
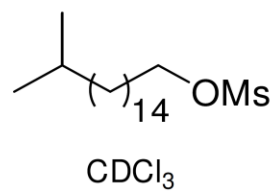
63.270  
39.222  
32.981  
30.105  
29.883  
29.852  
29.840  
29.832  
29.814  
29.772  
29.756  
29.592  
28.128  
27.577  
25.896  
22.816



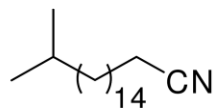
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – 16-Methylheptadecyl methanesulfonate (**26**)



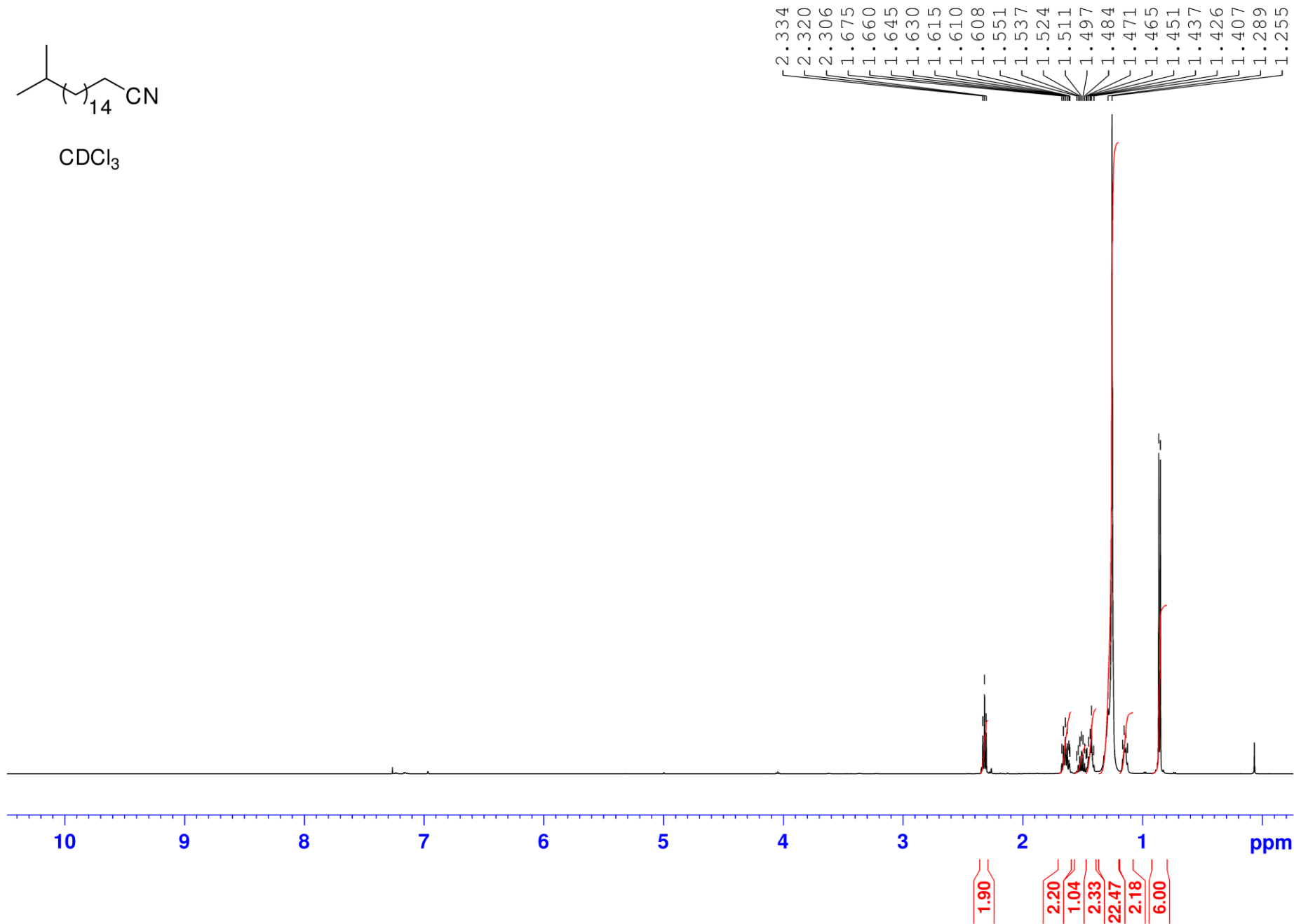
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 16-Methylheptadecyl methanesulfonate (**26**)



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) – 17-Methyloctadecanenitrile (**27**)

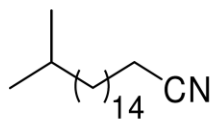


$\text{CDCl}_3$





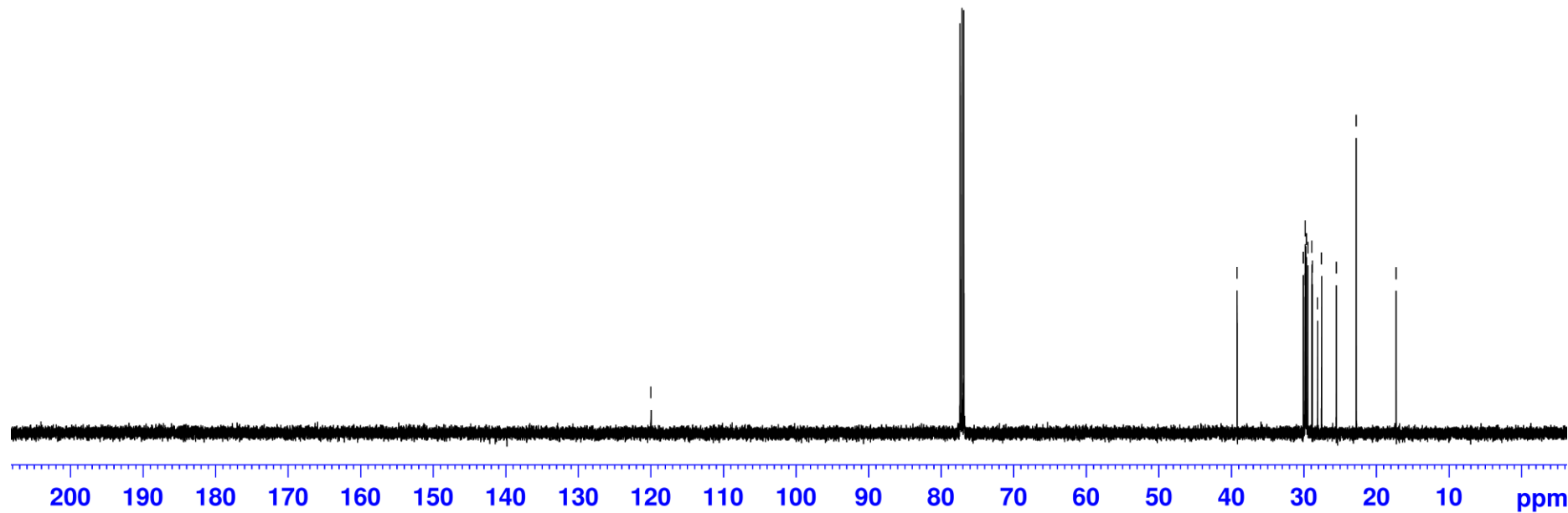
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 17-Methyloctadecanenitrile (**27**)



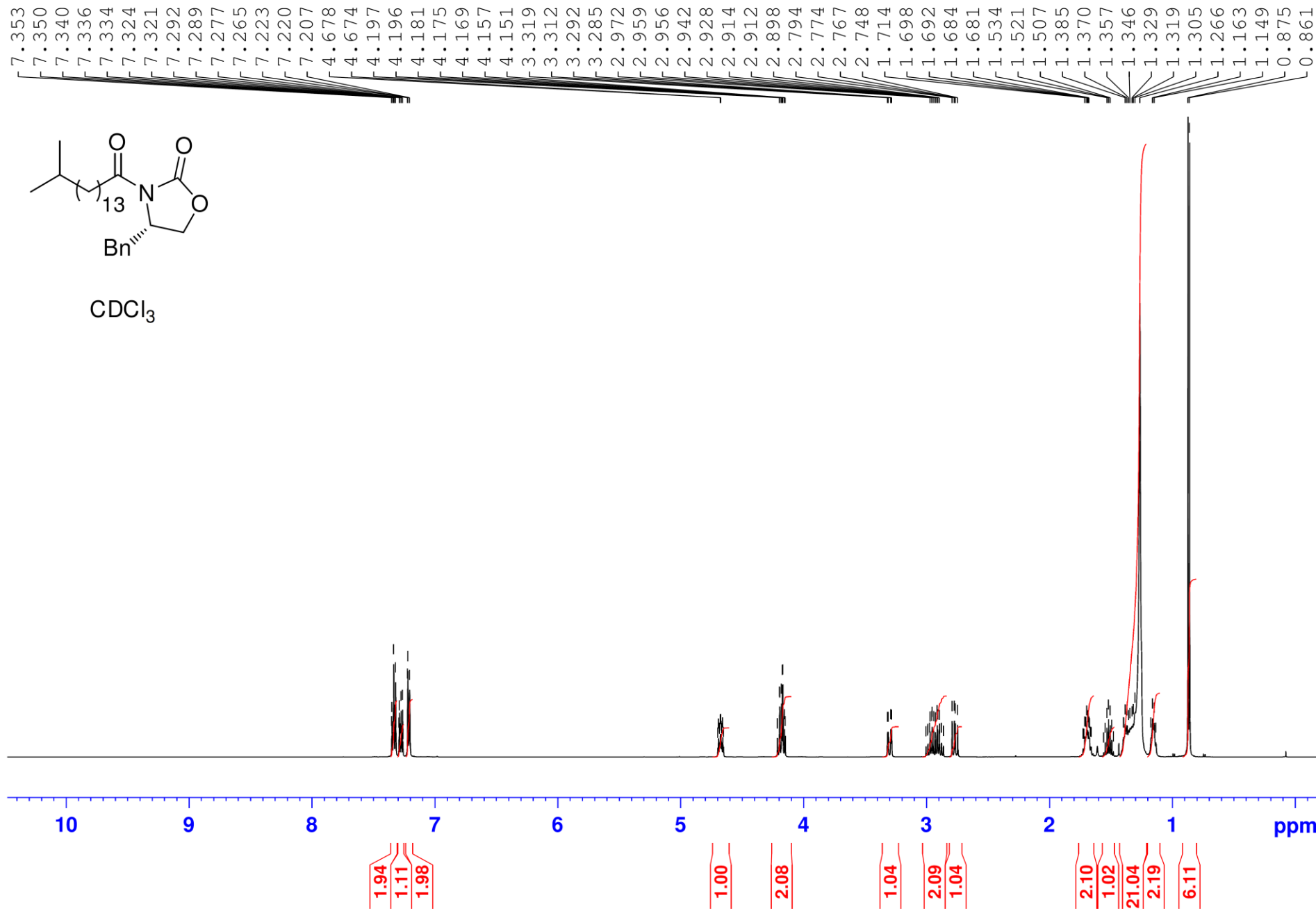
$\text{CDCl}_3$

—120.012

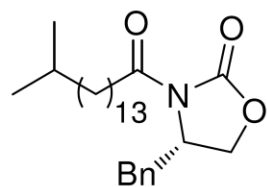
39.218  
30.100  
29.878  
29.843  
29.836  
29.817  
29.789  
29.742  
29.654  
29.456  
28.919  
28.824  
28.125  
27.573  
25.534  
22.814  
17.283



<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – (S)-4-Benzyl-3-(15-methylhexadecanoyl)oxazolidin-2-one (**28**)



<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) – (S)-4-Benzyl-3-(15-methylhexadecanoyl)oxazolidin-2-one (**28**)



CDCl<sub>3</sub>

— 173.569

— 153.577

— 135.473

— 129.549

— 129.069

— 127.454

— 77.414

— 77.160

— 76.906

— 66.265

— 55.281

— 39.192

— 38.071

— 35.671

— 30.081

— 29.860

— 29.824

— 29.817

— 29.796

— 29.754

— 29.628

— 29.537

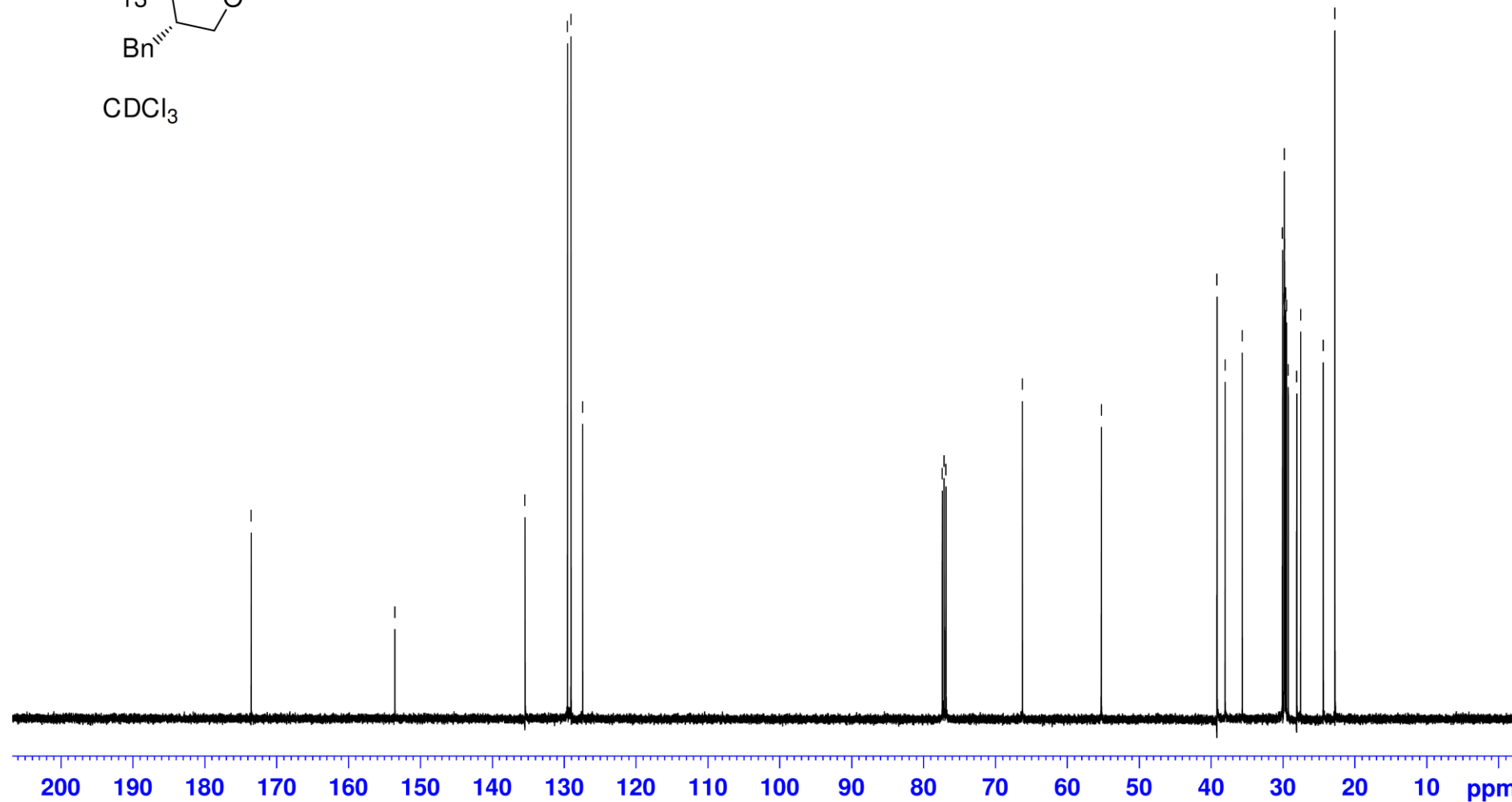
— 29.276

— 28.098

— 27.554

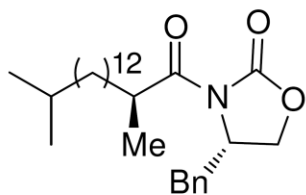
— 24.412

— 22.795

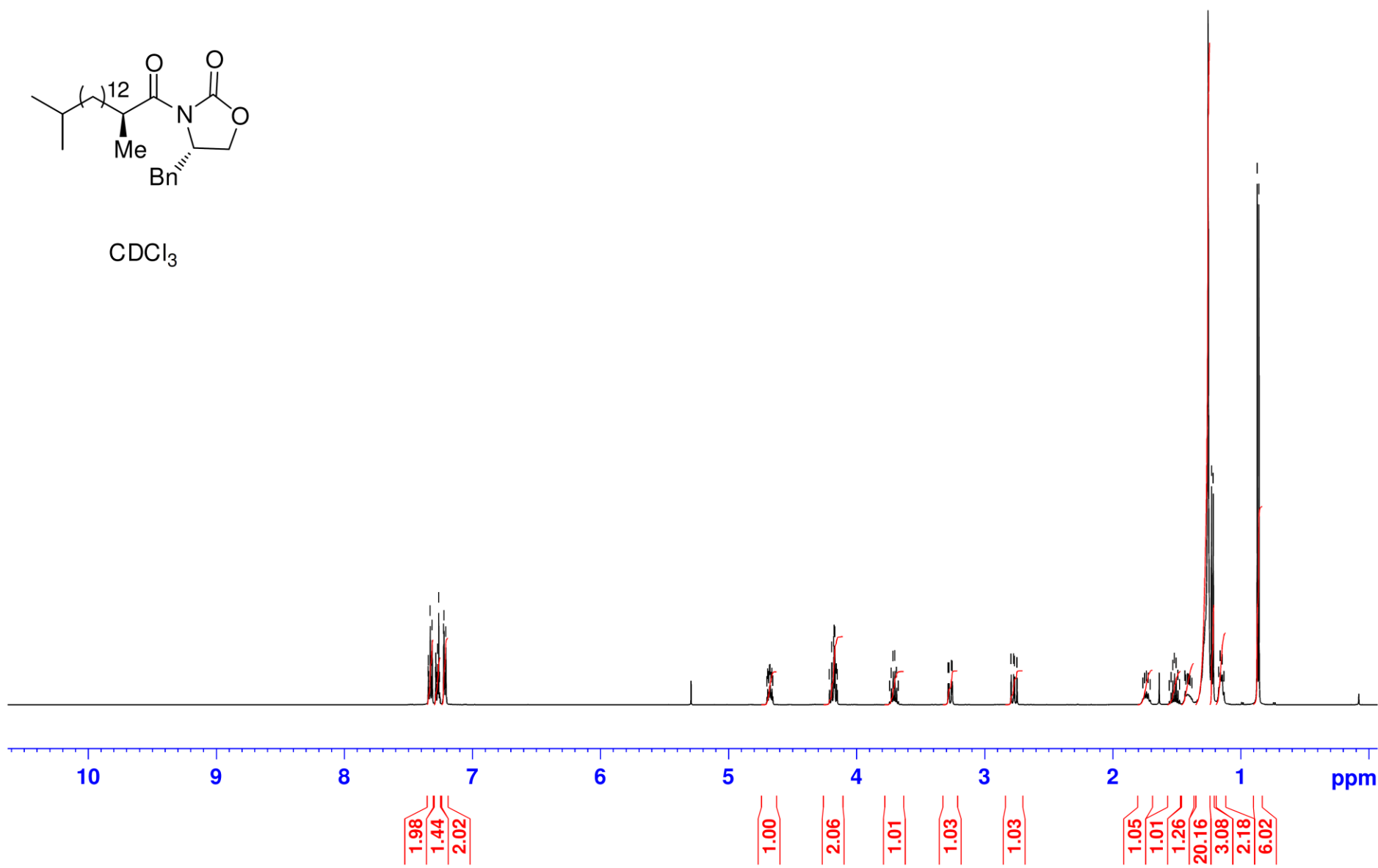


<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) – (S)-4-Benzyl-3-((S)-2,15-dimethylhexadecanoyl)oxazolidin-2-one (**29**)

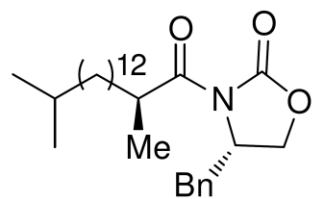
7.347  
7.345  
7.342  
7.331  
7.328  
7.319  
7.316  
7.289  
7.287  
7.284  
7.277  
7.272  
7.265  
7.258  
7.227  
7.224  
7.210  
7.210  
4.696  
4.689  
4.681  
4.677  
4.670  
4.668  
4.662  
4.213  
4.195  
4.180  
4.176  
4.170  
4.158  
4.152  
3.730  
3.716  
3.703  
3.689  
3.287  
3.281  
3.260  
3.254  
2.795  
2.775  
2.768  
2.749  
1.738  
1.545  
1.532  
1.519  
1.506  
1.492  
1.437  
1.257  
1.230  
1.216  
1.174  
1.161  
1.147  
1.133  
0.873  
0.860



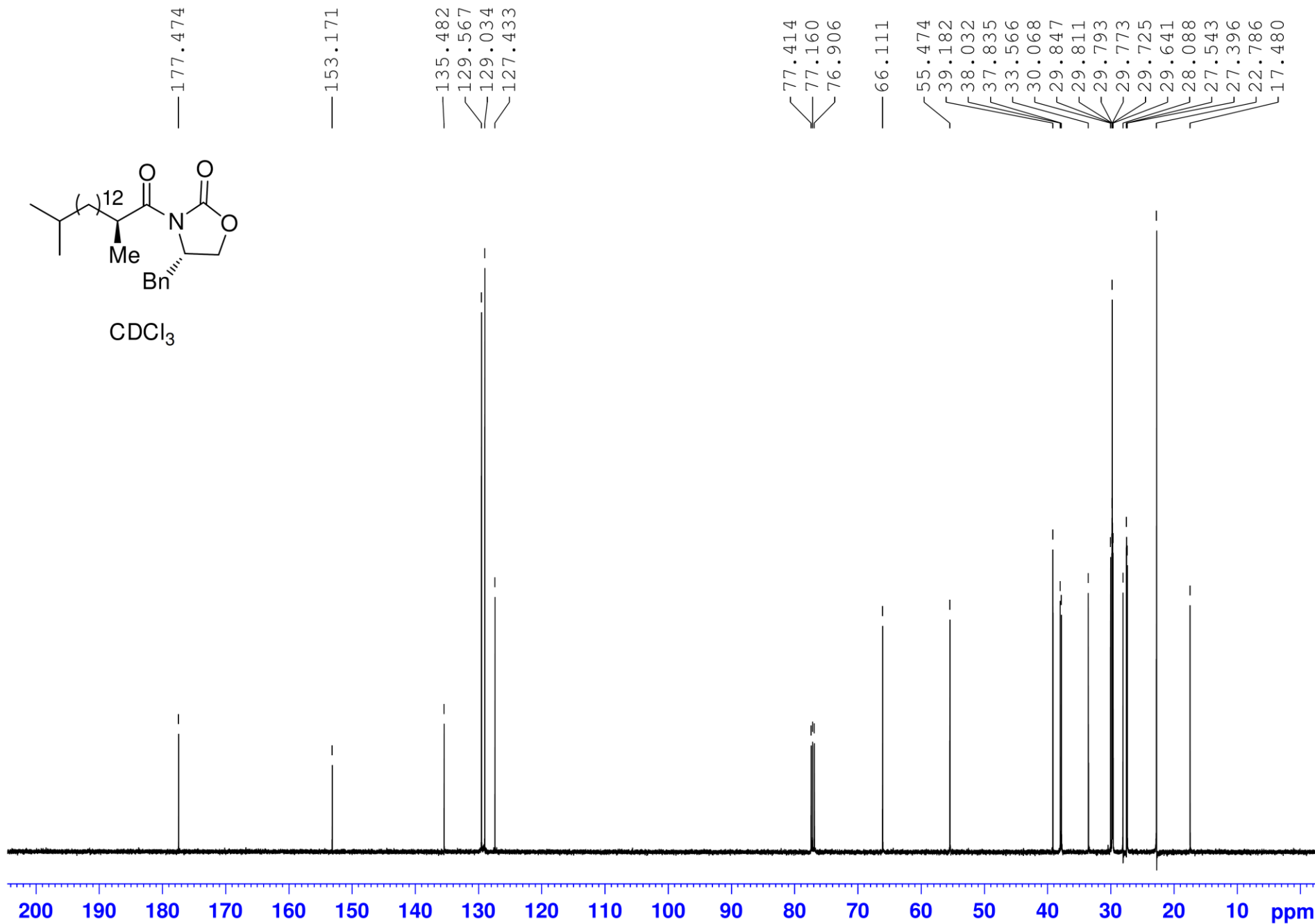
CDCl<sub>3</sub>



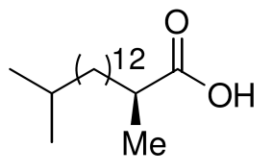
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – (S)-4-Benzyl-3-((S)-2,15-dimethylhexadecanoyl)oxazolidin-2-one (**29**)



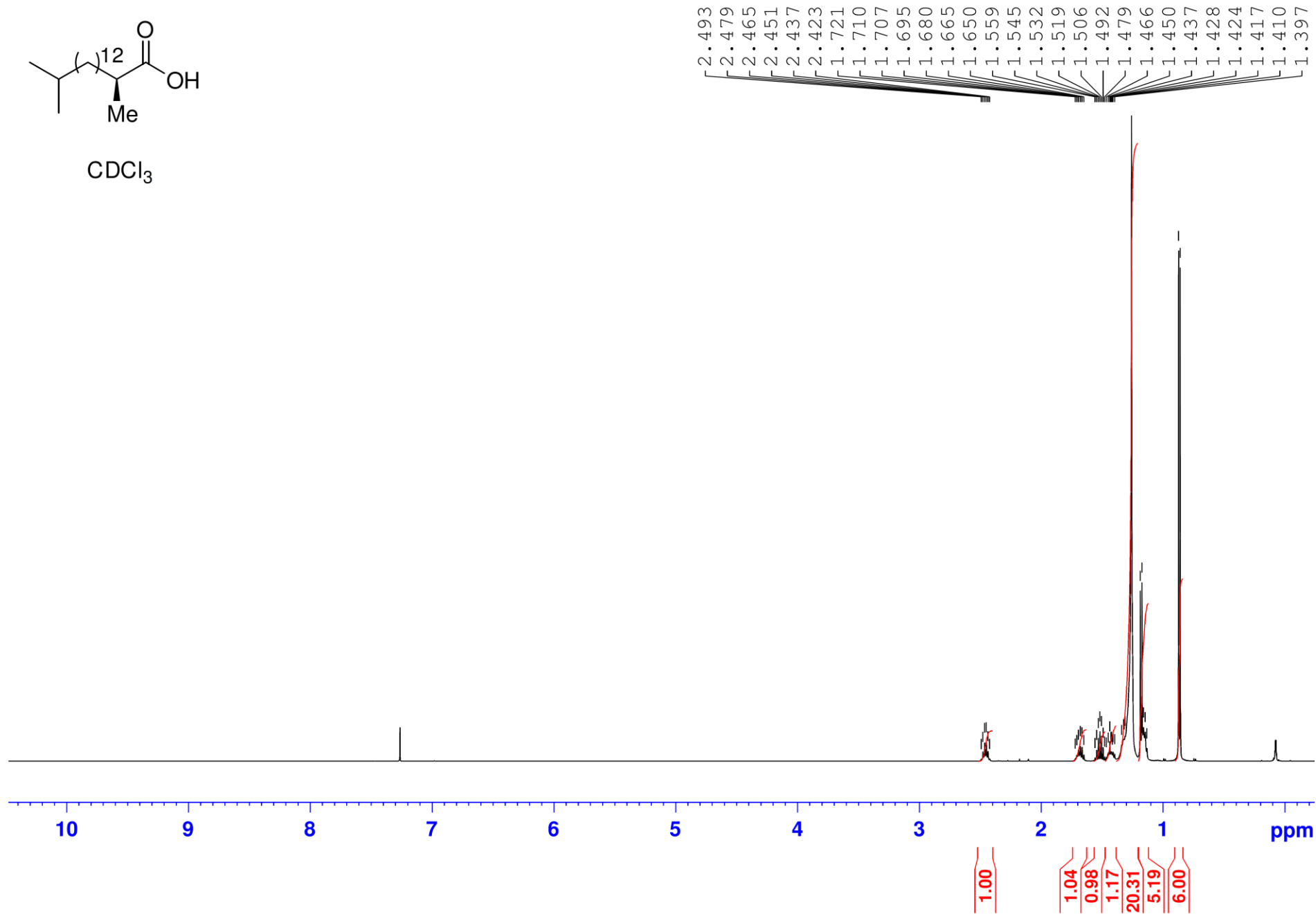
CDCl<sub>3</sub>



$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) – (*S*)-2,15-Dimethylhexadecanoic acid (**30**)



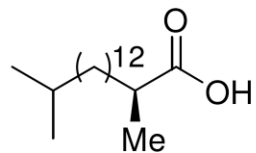
$\text{CDCl}_3$



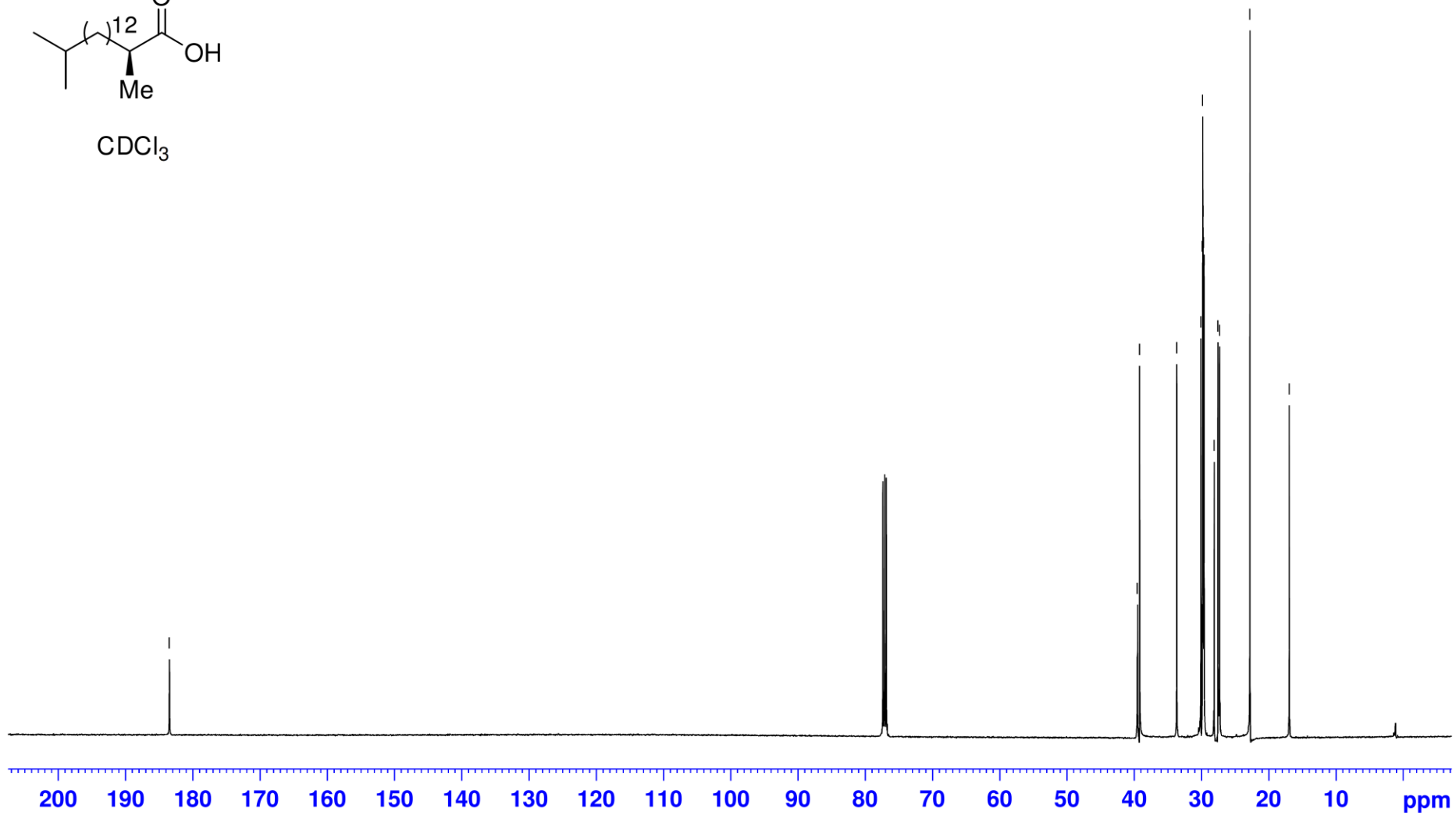
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – (*S*)-2,15-Dimethylhexadecanoic acid (**30**)

— 183.510

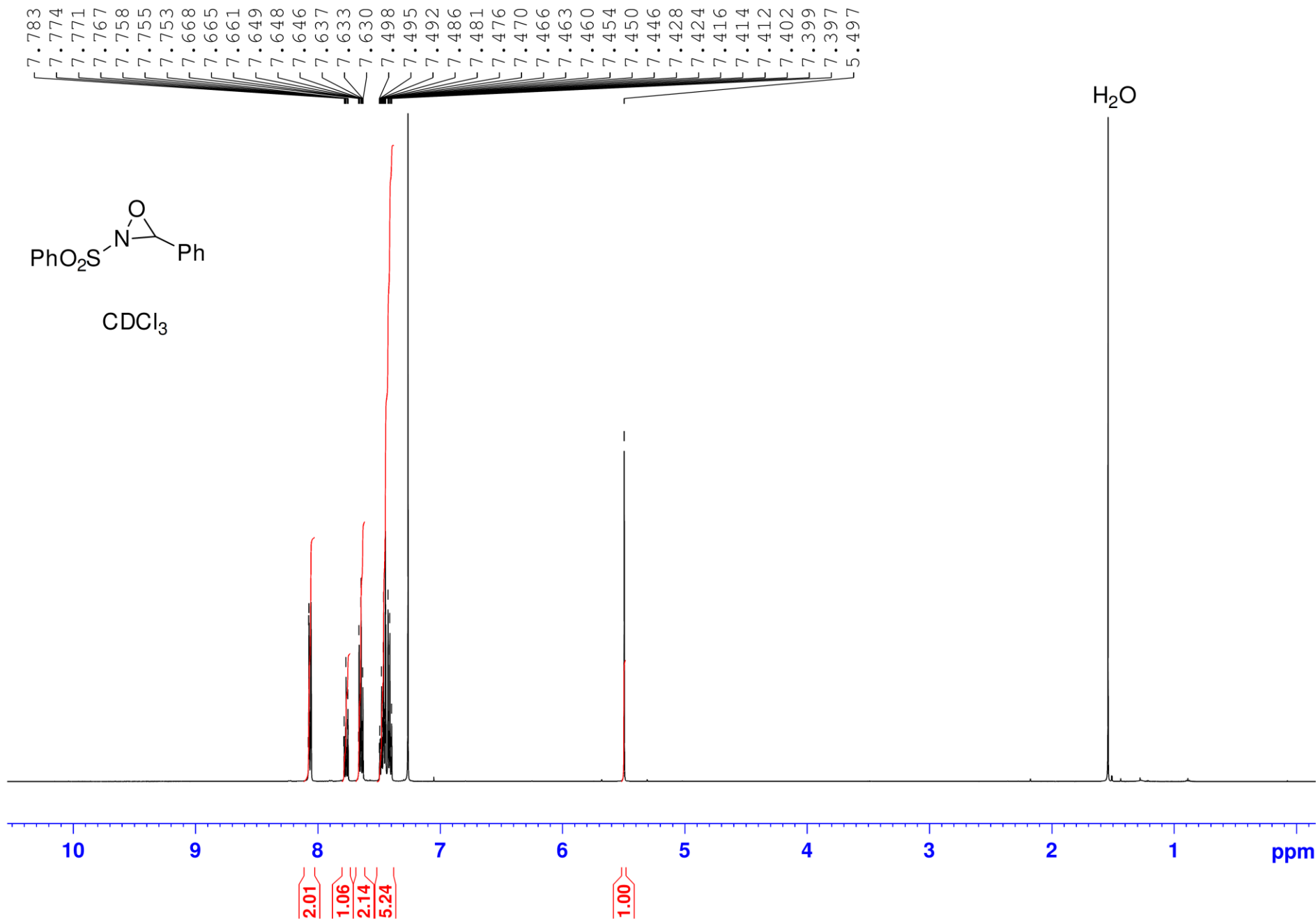
39.543  
39.224  
33.695  
30.110  
29.883  
29.849  
29.831  
29.805  
29.764  
29.673  
29.636  
28.130  
27.583  
27.308  
22.816  
16.971



$\text{CDCl}_3$

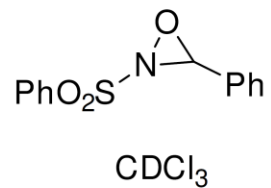


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – 3-Phenyl-2-(phenylsulfonyl)-1,2-oxaziridine





$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – 3-Phenyl-2-(phenylsulfonyl)-1,2-oxaziridine



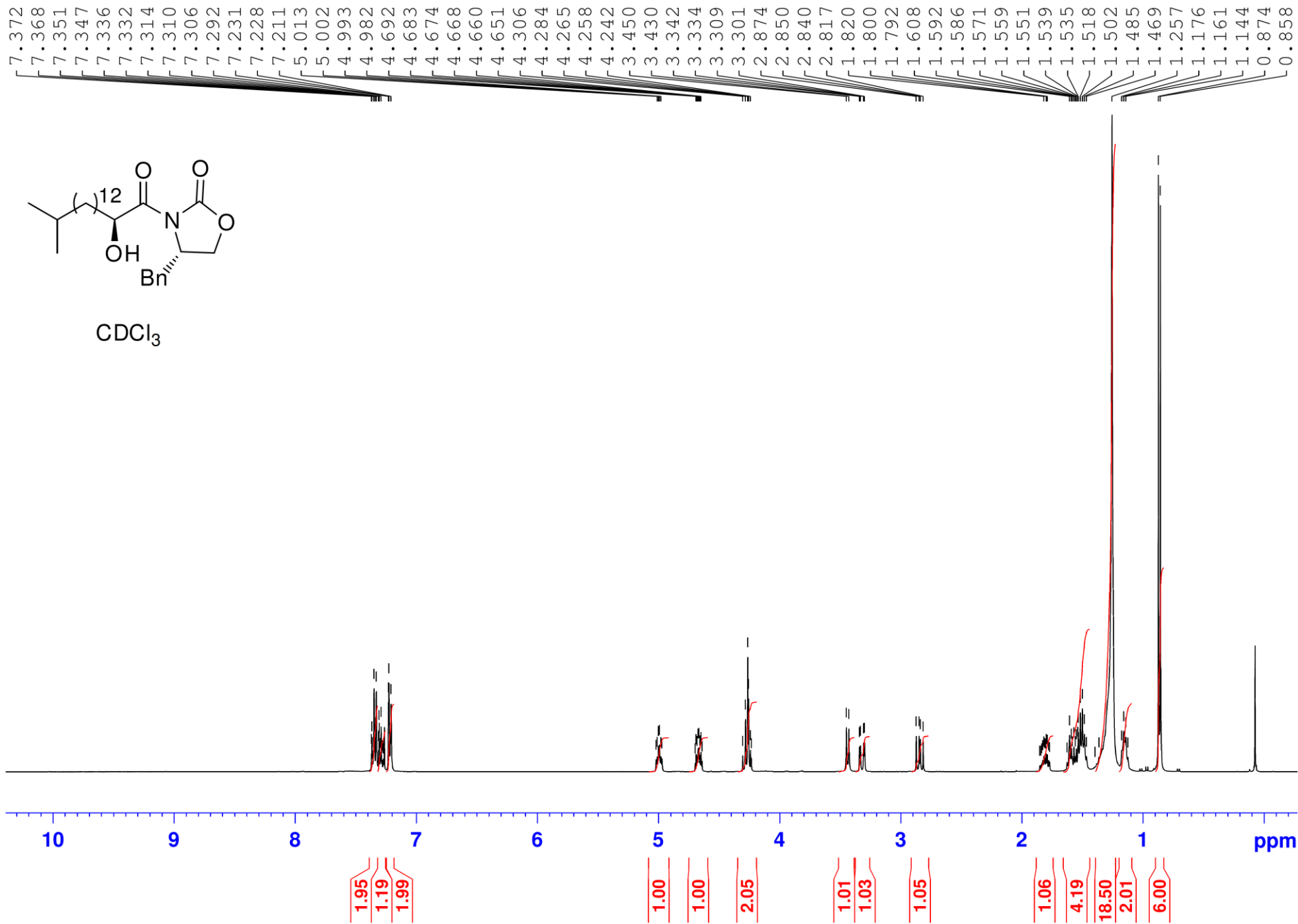
135.158  
134.907  
131.596  
130.621  
129.541  
129.526  
128.910  
128.405

76.449

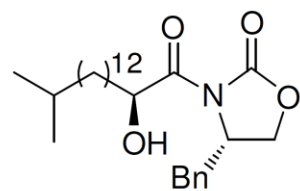


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm S57

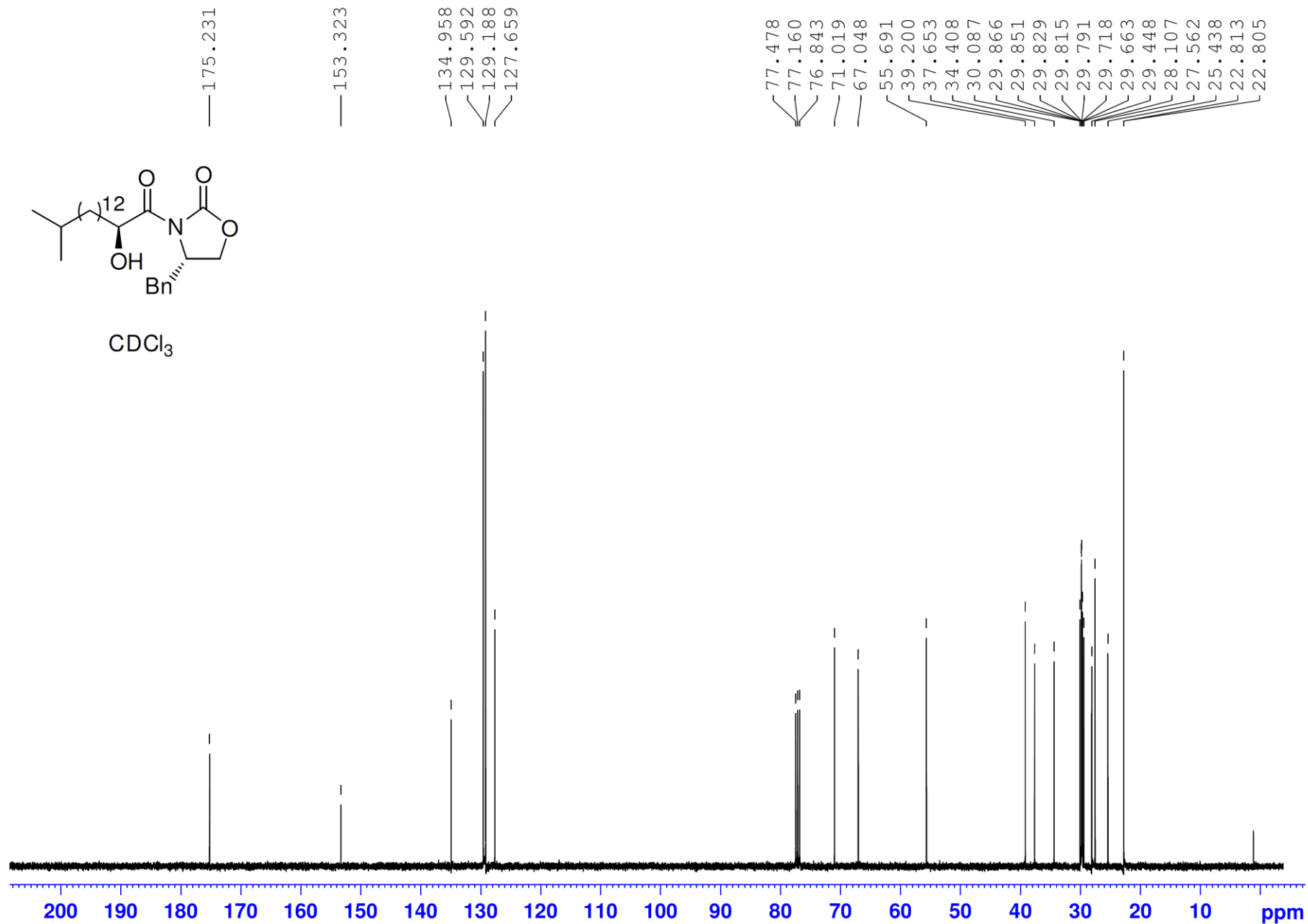
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – (S)-4-Benzyl-3-((S)-2-hydroxy-15-methylhexadecanoyl)oxazolidin-2-one (**31**)



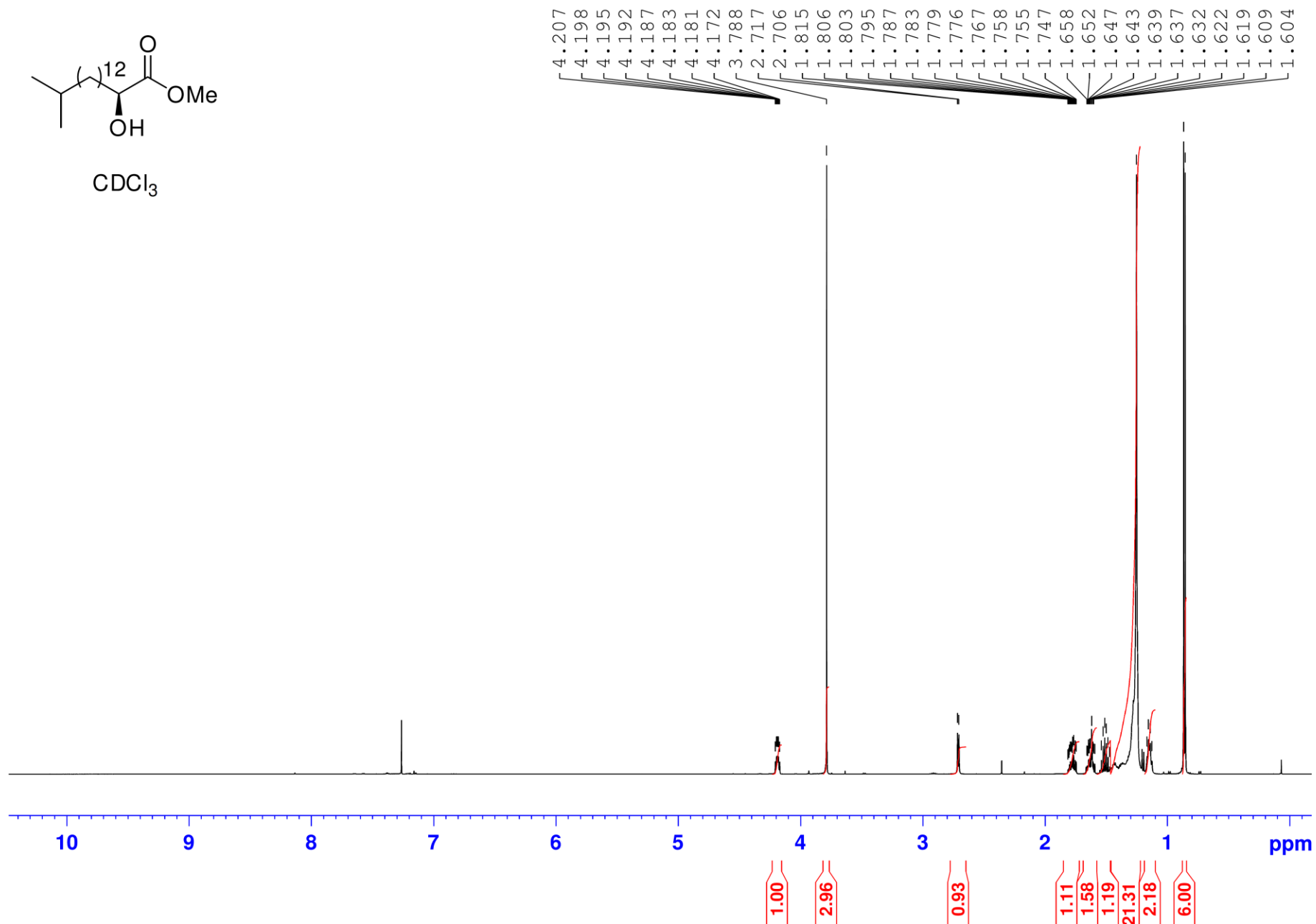
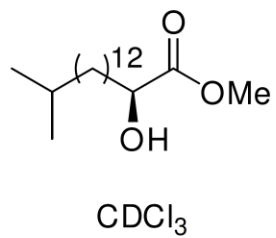
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) – (*S*)-4-Benzyl-3-((*S*)-2-hydroxy-15-methylhexadecanoyl)oxazolidin-2-one (**31**)



$\text{CDCl}_3$

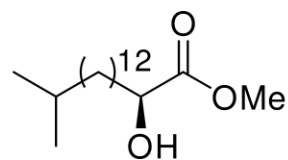


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – (S)-Methyl 2-hydroxy-15-methylhexadecanoate



<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) – (*S*)-Methyl 2-hydroxy-15-methylhexadecanoate

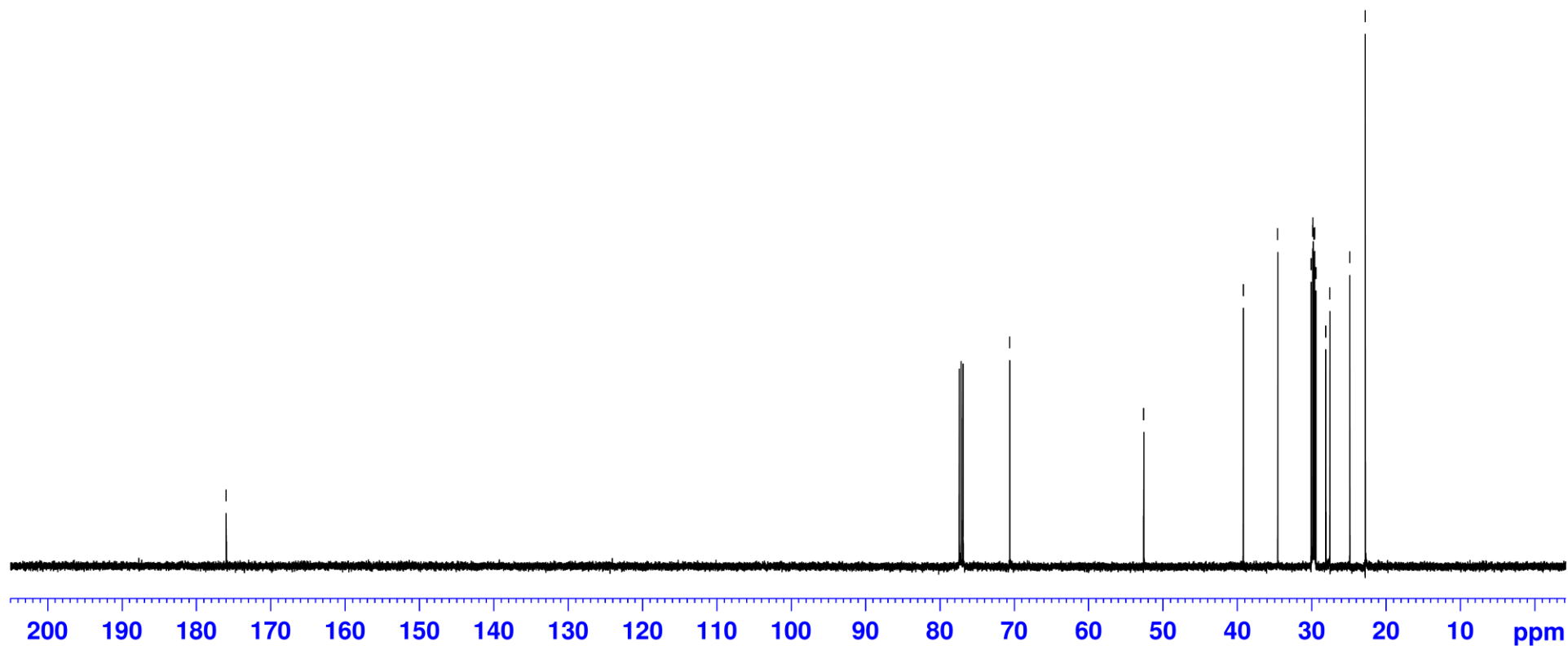
— 176.019



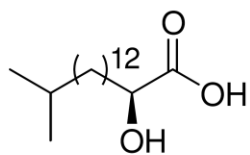
CDCl<sub>3</sub>

— 70.621

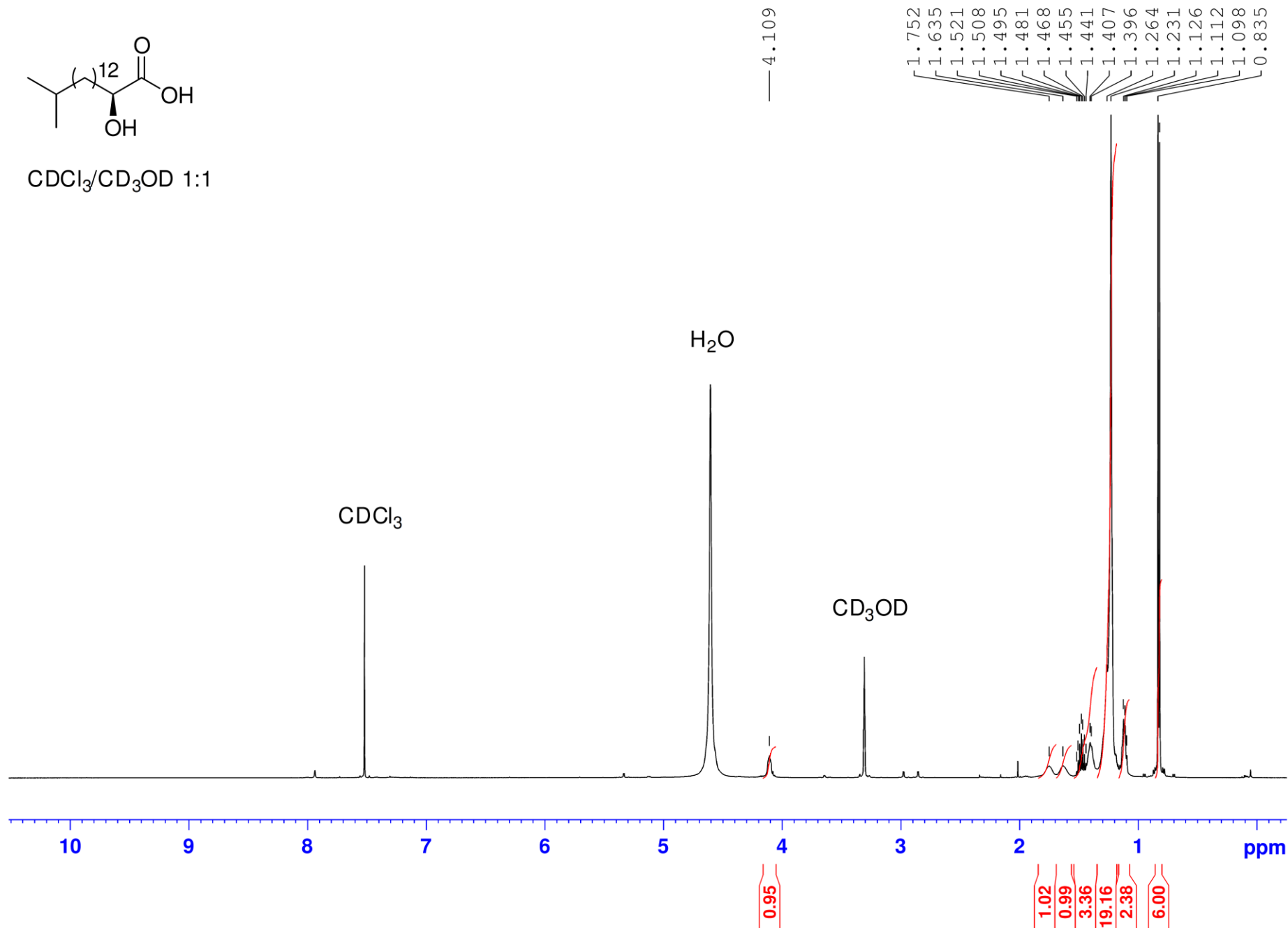
52.599  
39.208  
34.571  
30.089  
29.866  
29.828  
29.809  
29.773  
29.695  
29.601  
29.451  
28.114  
27.566  
24.884  
22.802



<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>/CD<sub>3</sub>OD) – (*S*)-2-Hydroxy-15-methylhexadecanoic acid (**32**)



CDCl<sub>3</sub>/CD<sub>3</sub>OD 1:1

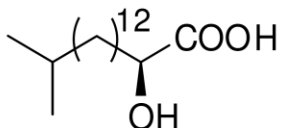


<sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>/TFA) – (*S*)-2-Hydroxy-15-methylhexadecanoic acid (**32**)

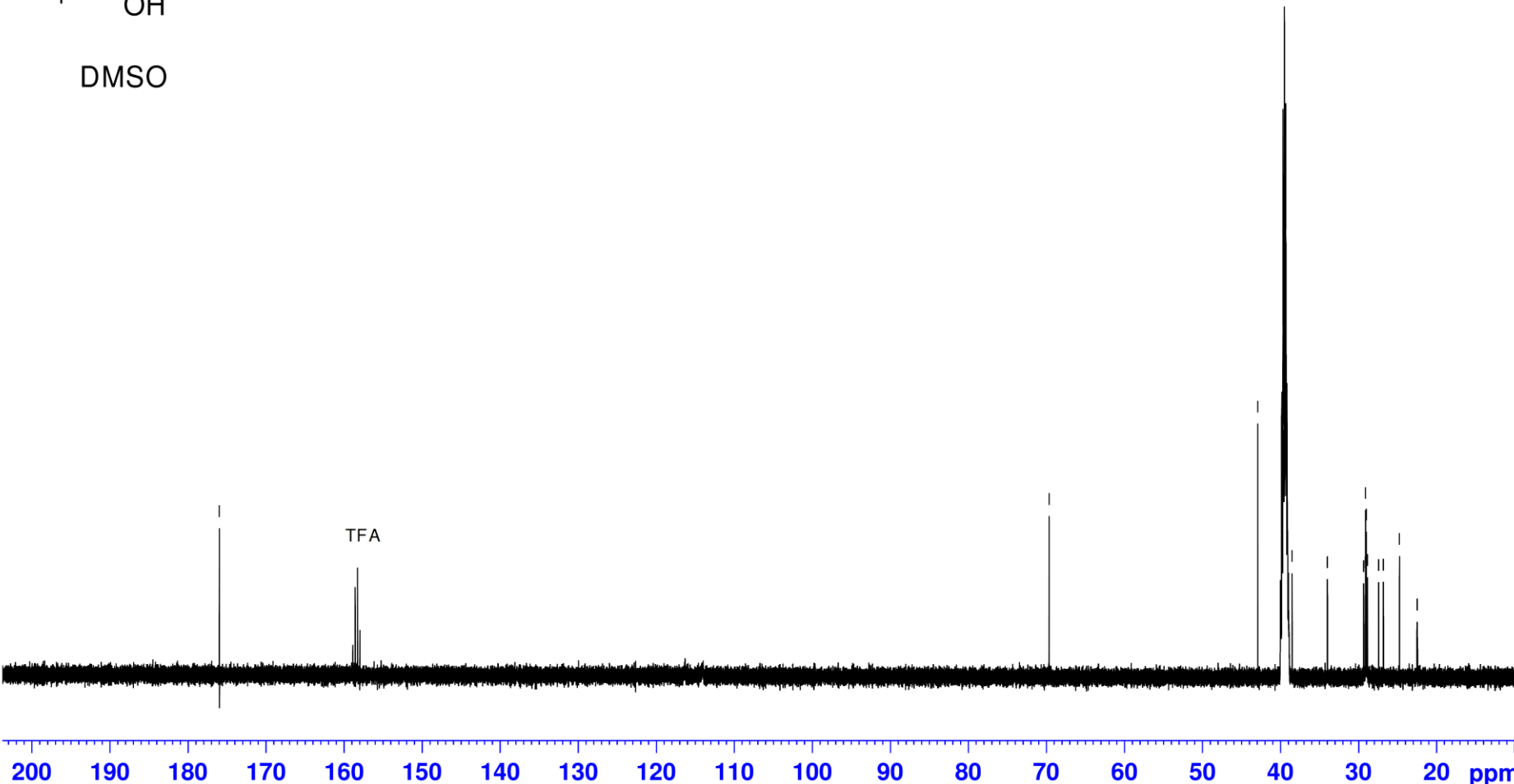
— 176.004

— 69.662

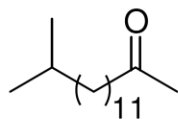
42.925  
38.530  
34.000  
29.361  
29.130  
29.103  
29.087  
29.045  
29.034  
28.867  
27.443  
26.835



DMSO

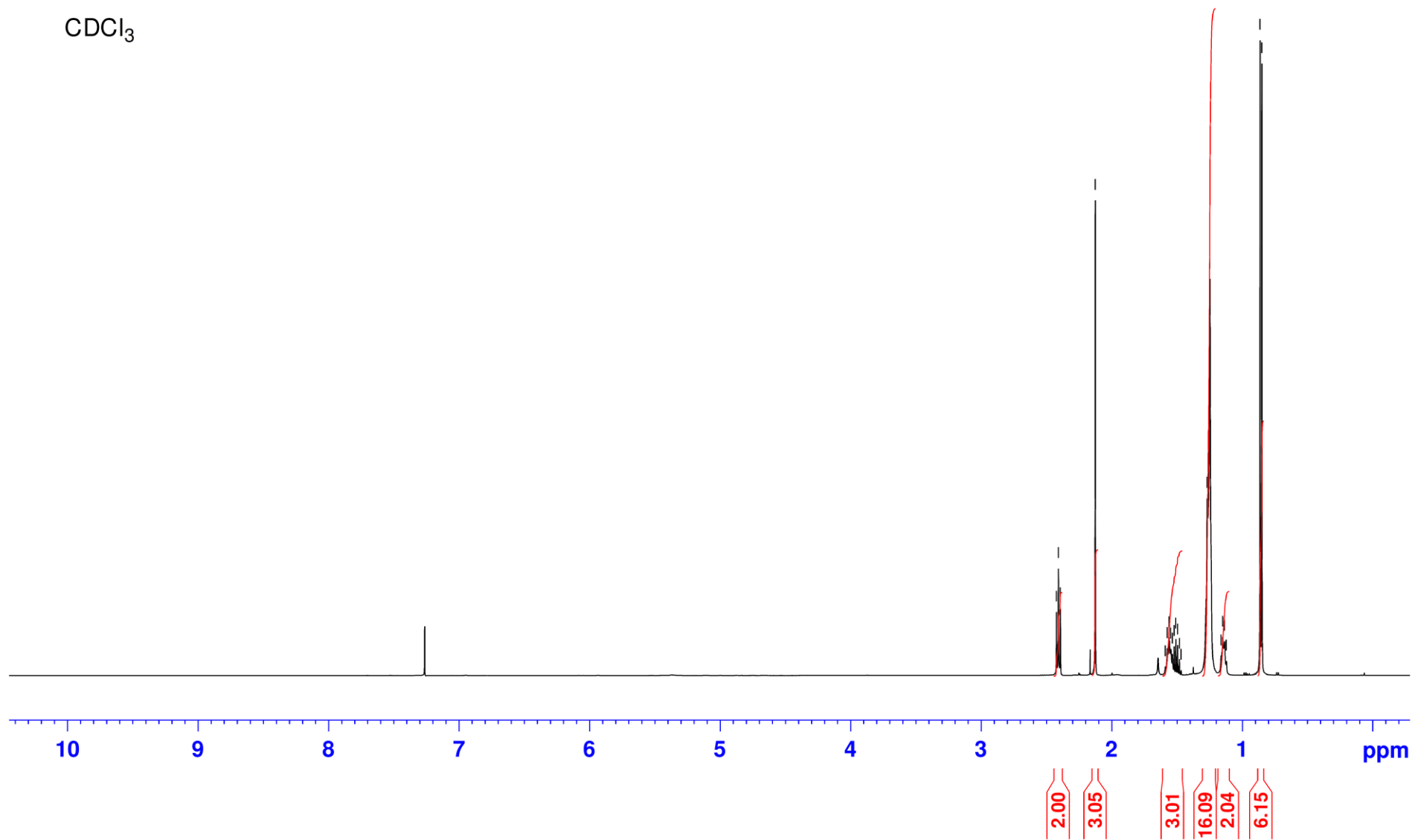


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) – 14-Methylpentadecan-2-one (**33**)



CDCl<sub>3</sub>

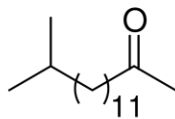
2.424  
2.410  
2.394  
2.128  
1.591  
1.576  
1.562  
1.549  
1.536  
1.523  
1.510  
1.496  
1.483  
1.470  
1.270  
1.250  
1.164  
1.151  
1.137  
1.123





<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) – 14-Methylpentadecan-2-one (**33**)

— 209.525



CDCl<sub>3</sub>

43.968  
39.196  
30.072  
29.971  
29.839  
29.787  
29.745  
29.608  
29.541  
29.327  
28.106  
27.551  
24.021  
22.794

