Supplementary Material

Spirocyclization reactions and antiproliferative activity of indole phytoalexins 1-methoxybrassinin and its 1-substituted derivatives

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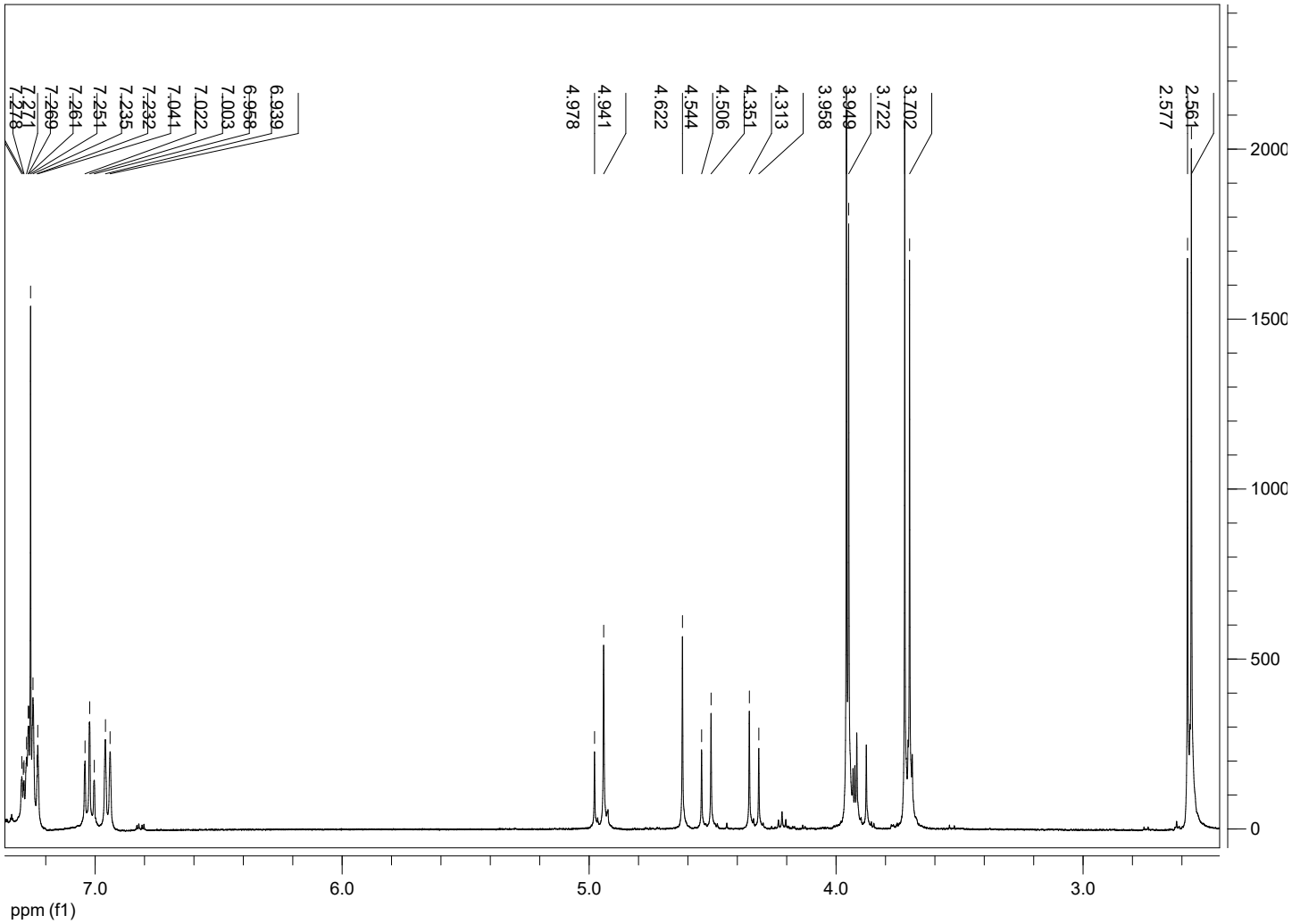
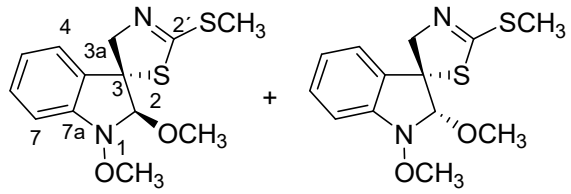
1. Experimental section

^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were measured on a Varian Mercury Plus spectrometer.

trans-(±)- and _cis_-(±)-1-Methoxyspirobrassinol methyl ether [_trans_-(±)-4a and _cis_-(±)-4b]

^{1}H NMR spectrum of mixture ***trans*-(±)-4a and *cis*-(±)-4b** in $CDCl_3$

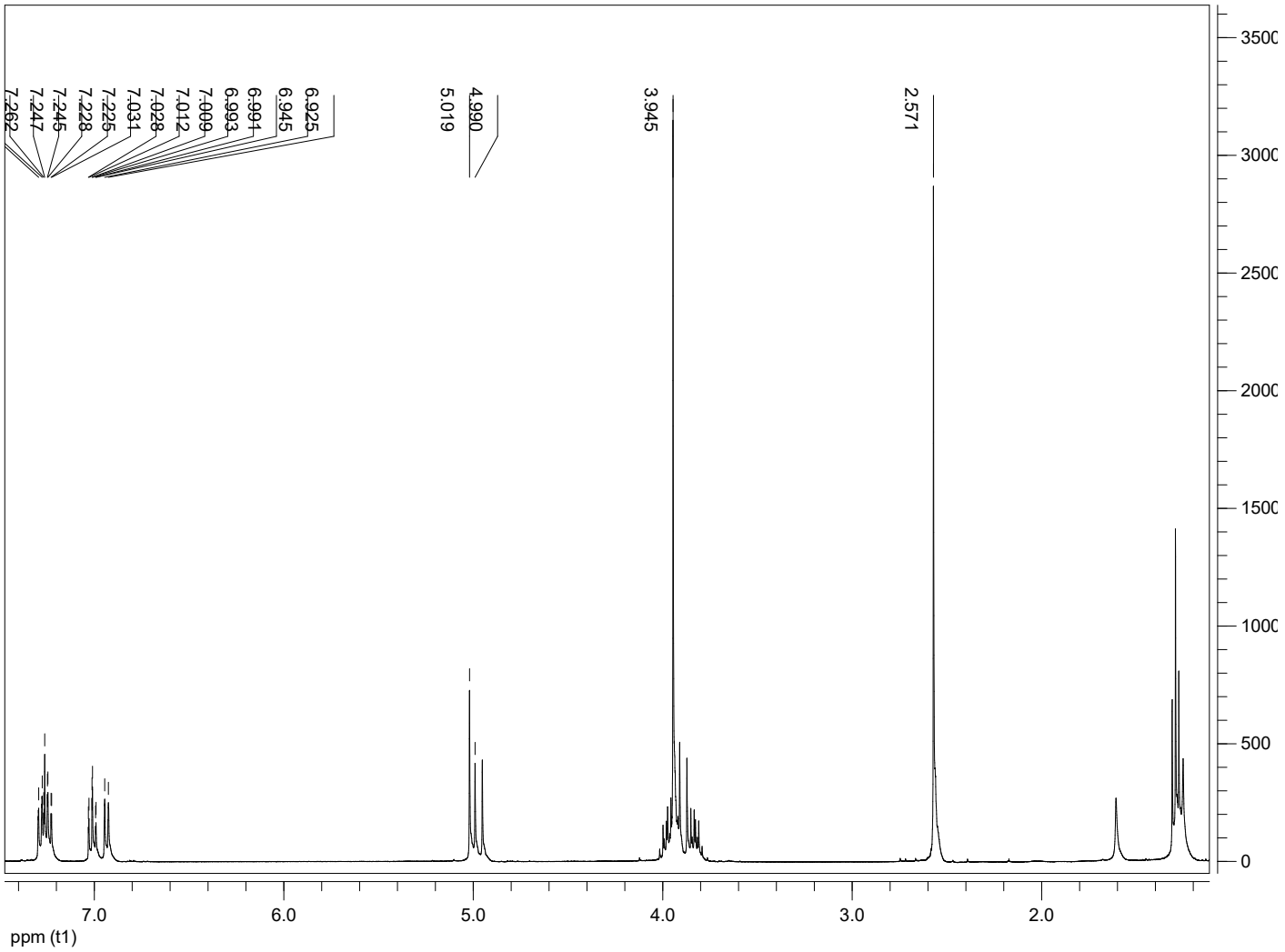


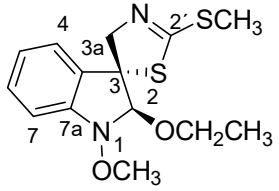


trans-(±)-**4a** *cis*-(±)-**4b**

trans-(±)-1-Methoxyspirobrassinol ethyl ether [_trans_-(±)-7a]

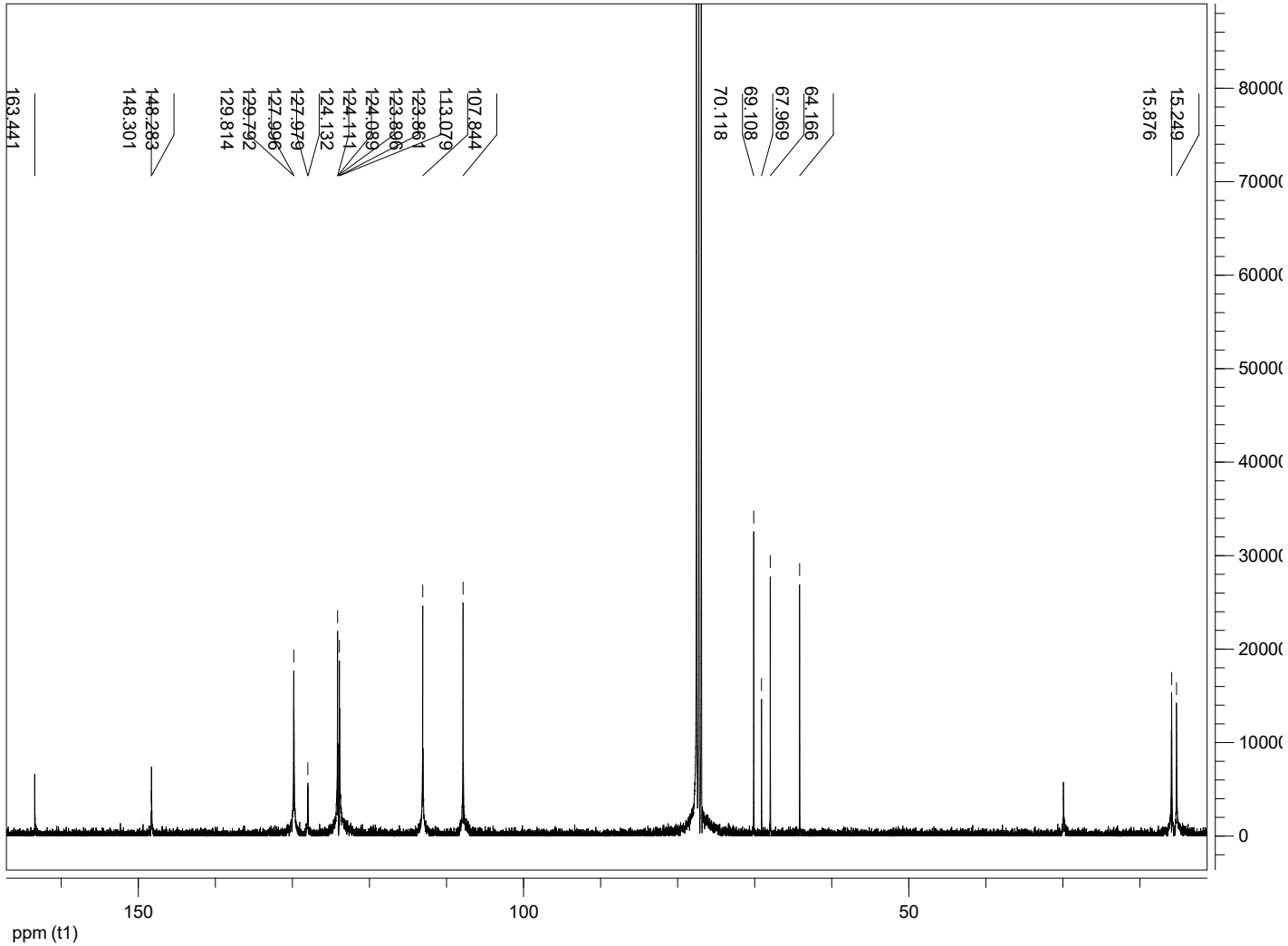
^{1}H NMR spectrum of ***trans*-(±)-7a** in $CDCl_3$





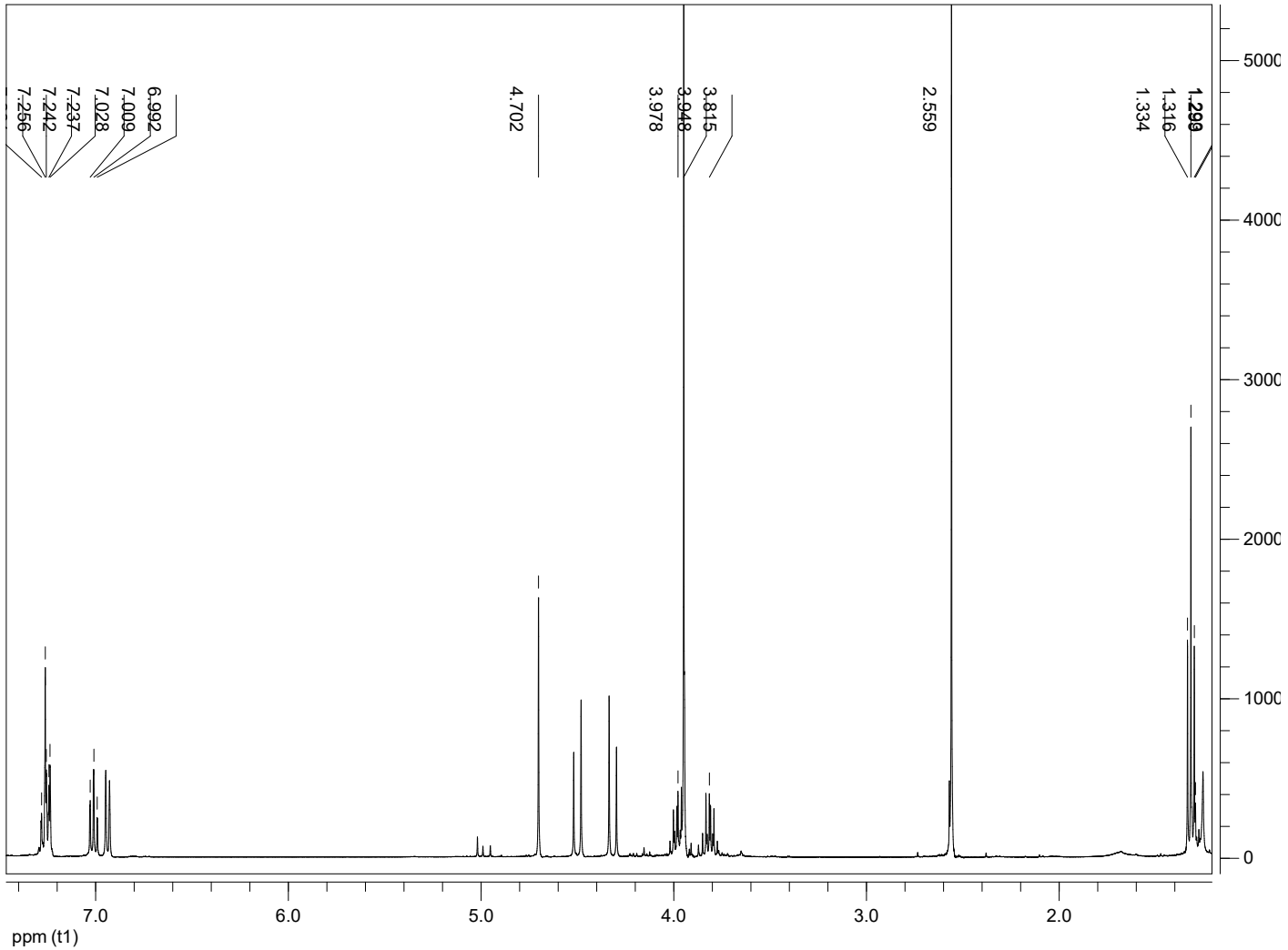
trans-(±)-**7a**

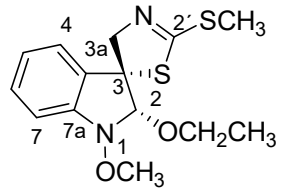
^{13}C NMR spectrum of ***trans*-(±)-7a** in $CDCl_3$



cis-(±)-1-Methoxyspirobrassinol ethyl ether [_cis_-(±)-7b]

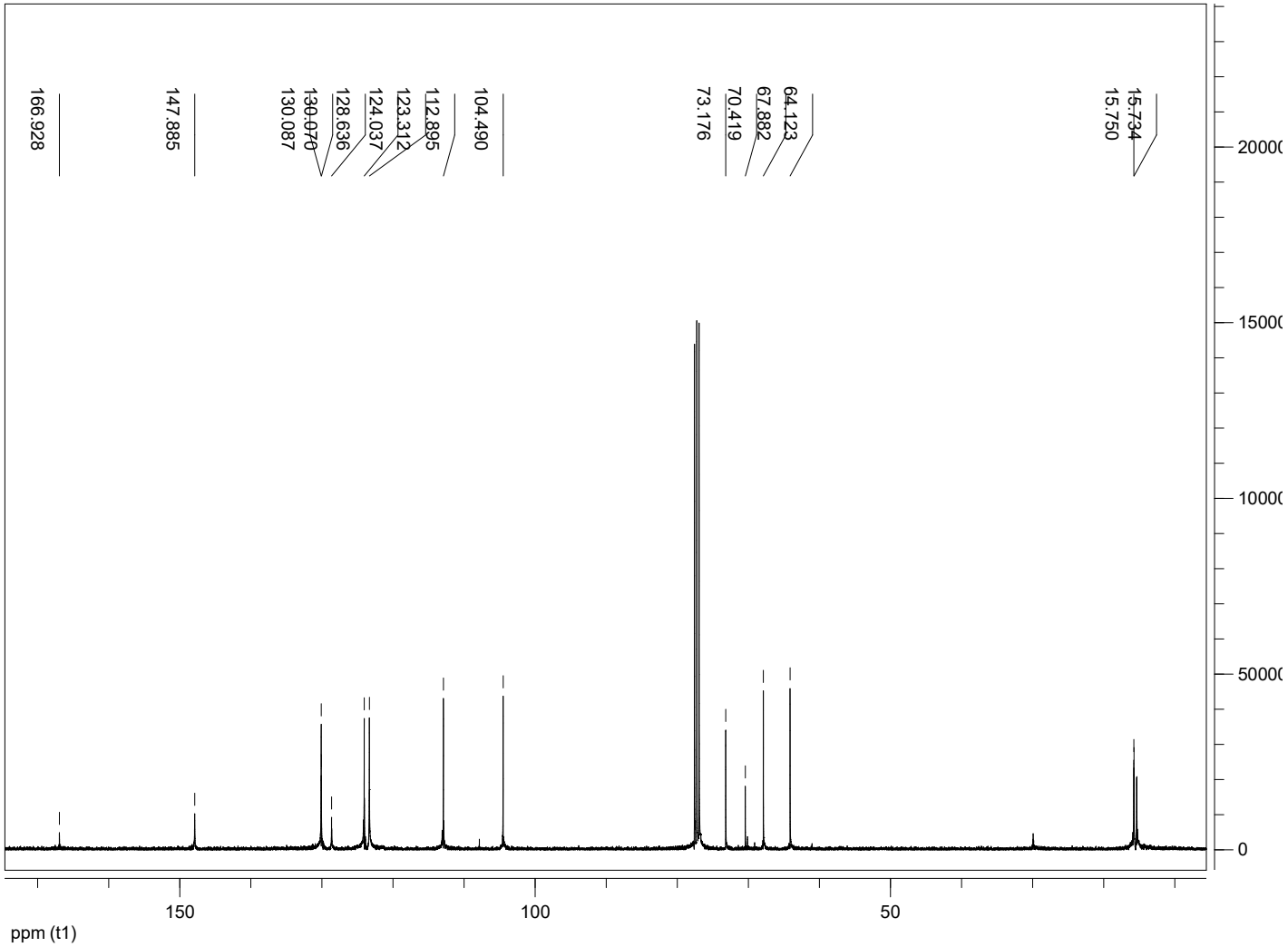
^{1}H NMR spectrum of ***cis*-(±)-7b** in $CDCl_3$





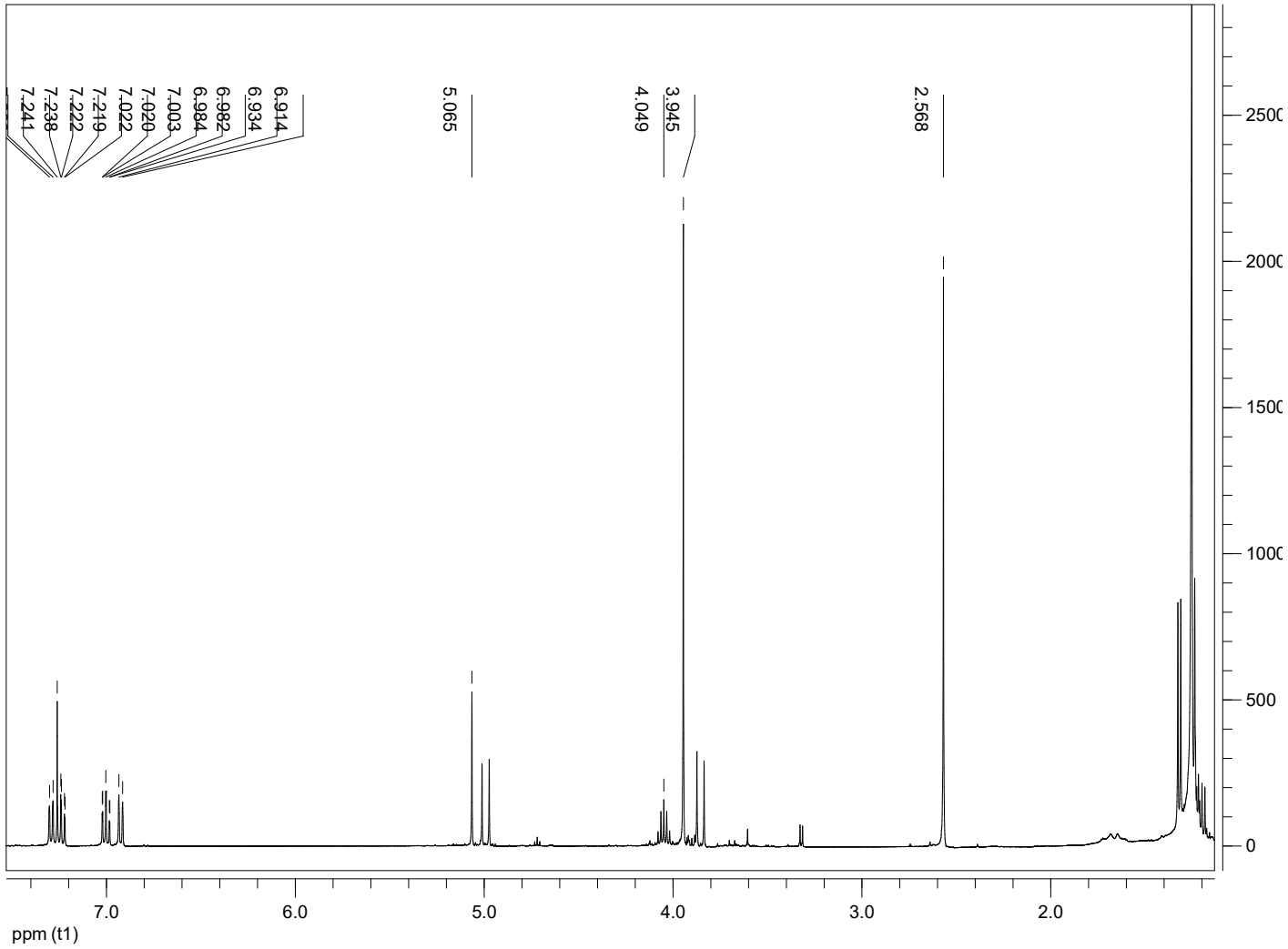
***cis*-(±)-7b**

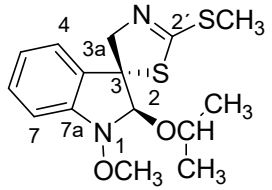
^{13}C NMR spectrum of ***cis*-(±)-7b** in $CDCl_3$



trans-(±)-1-Methoxyspirobrassinol isopropyl ether [_trans_-(±)-8a]

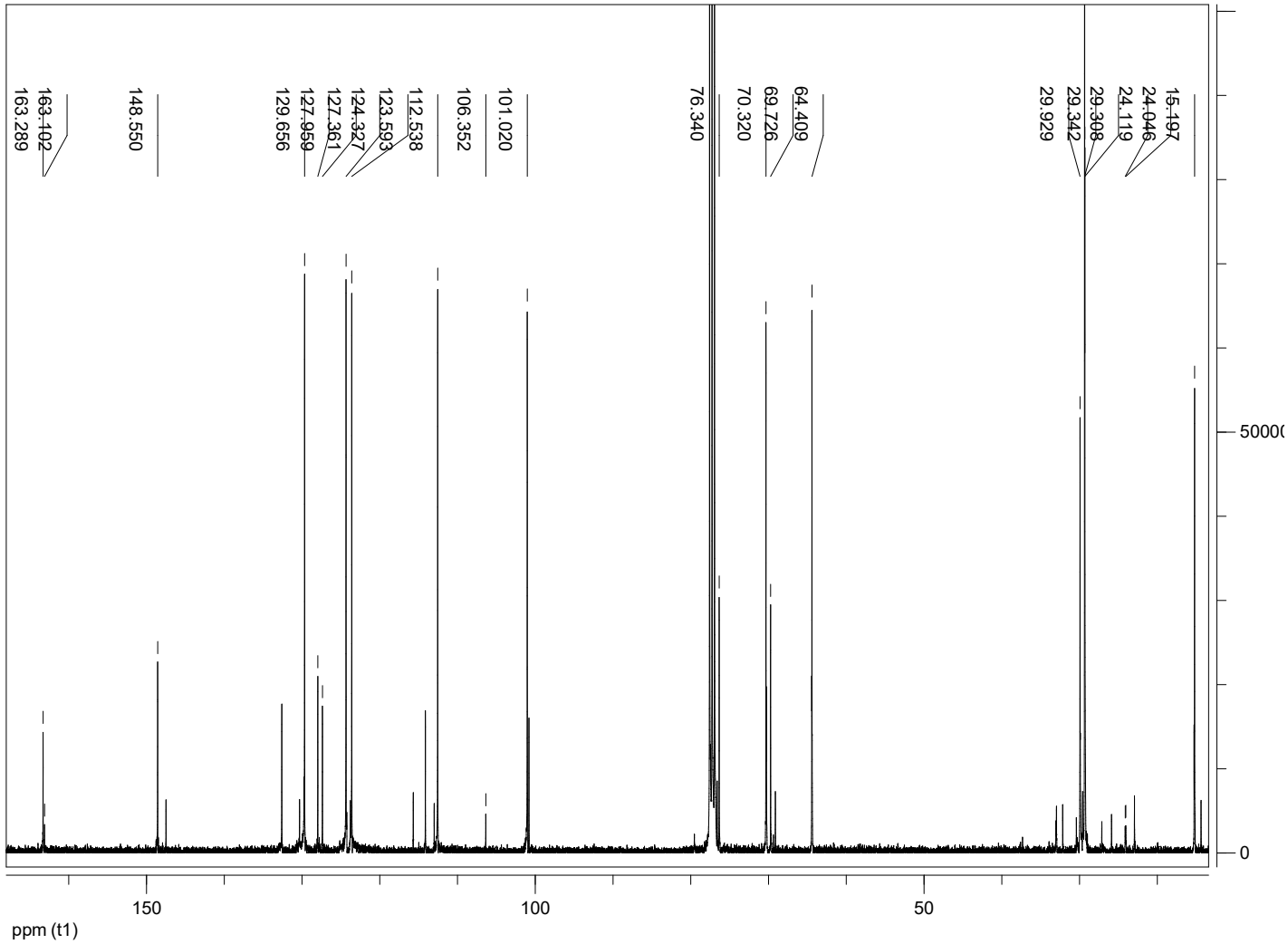
^{1}H NMR spectrum of ***trans*-(±)-8a** in $CDCl_3$





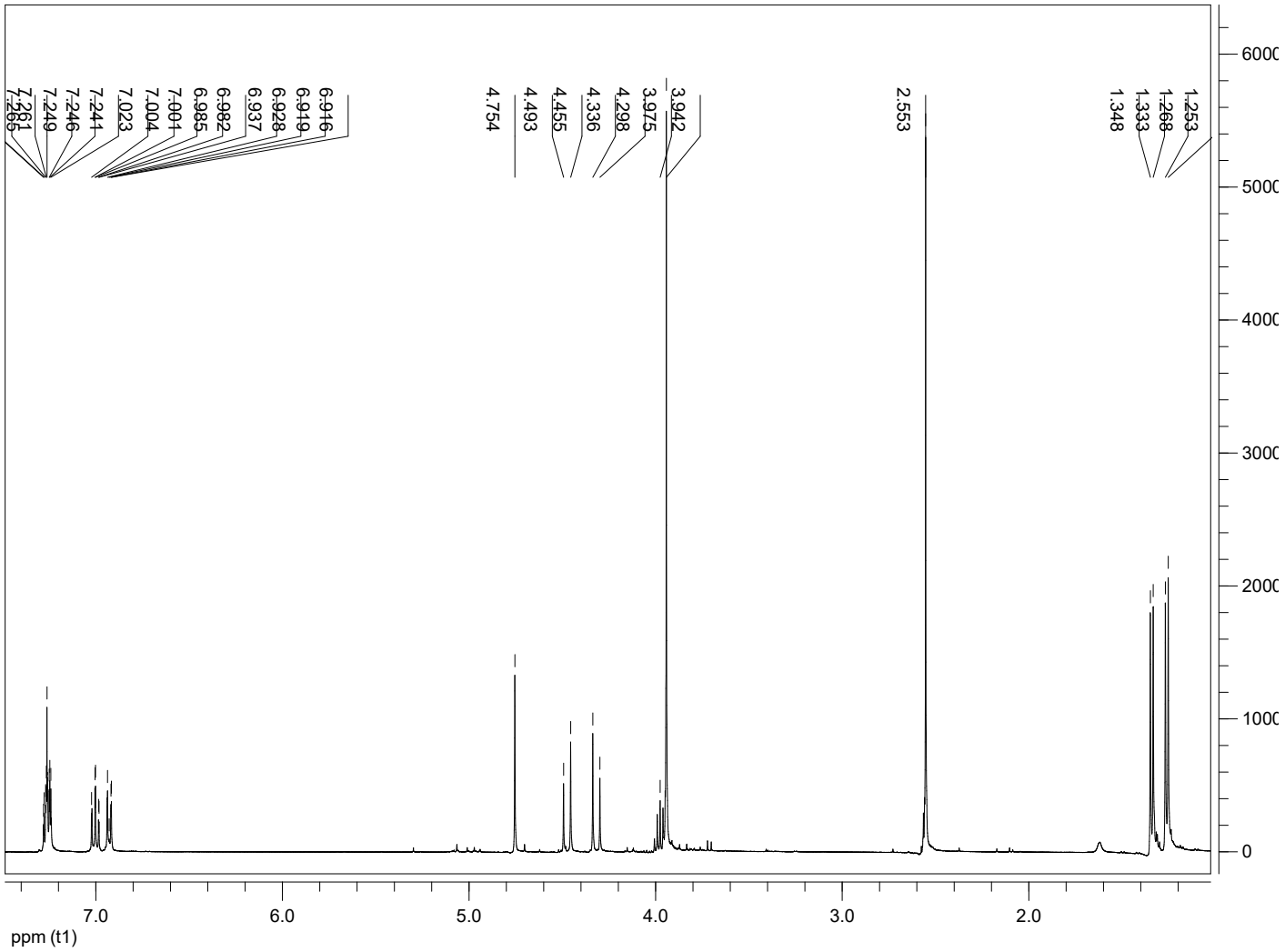
trans-(±)-**8a**

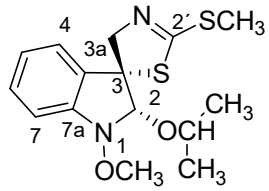
^{13}C NMR spectrum of ***trans*-(±)-8a** in $CDCl_3$



cis-(±)-1-Methoxyspirobrassinol isopropyl ether [_cis_-(±)-8b]

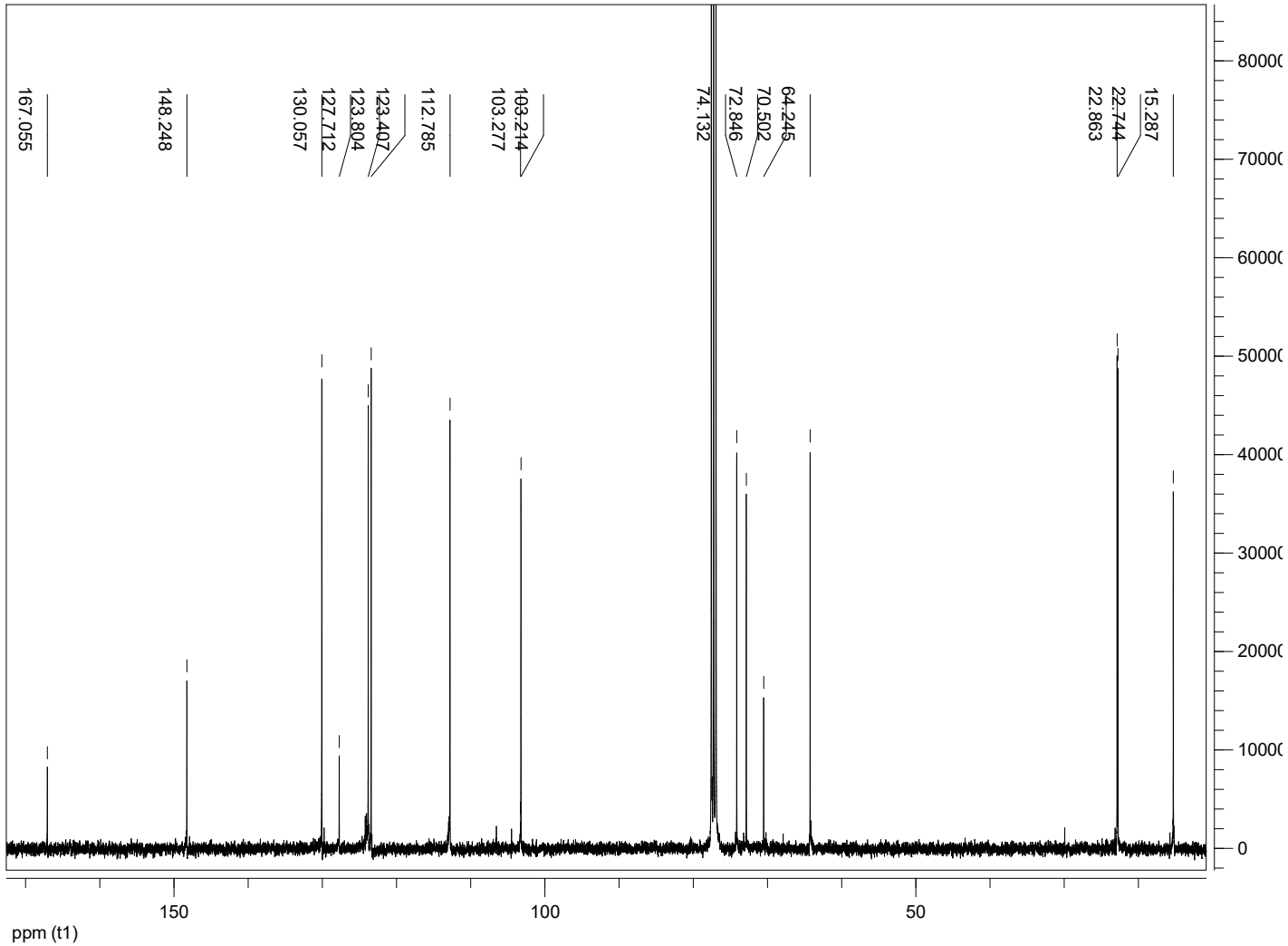
^{1}H NMR spectrum of ***cis*-(±)-8b** in $CDCl_3$





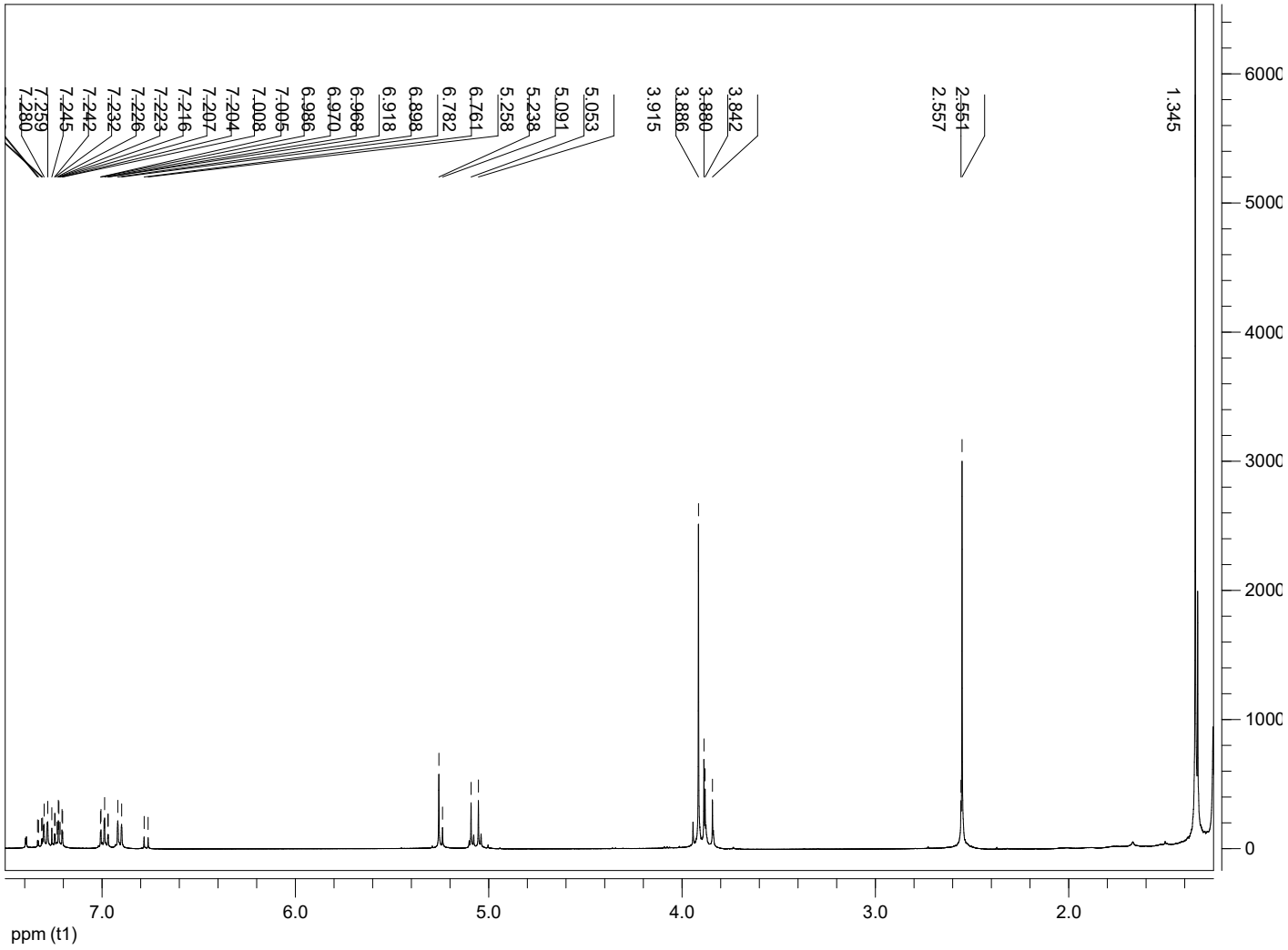
***cis*-(±)-8b**

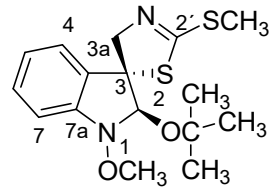
^{13}C NMR spectrum of ***cis*-(±)-8b** in $CDCl_3$



trans-(±)-1-Methoxyspirobrassinol _tert_-butyl ether [_trans_-(±)-9a]

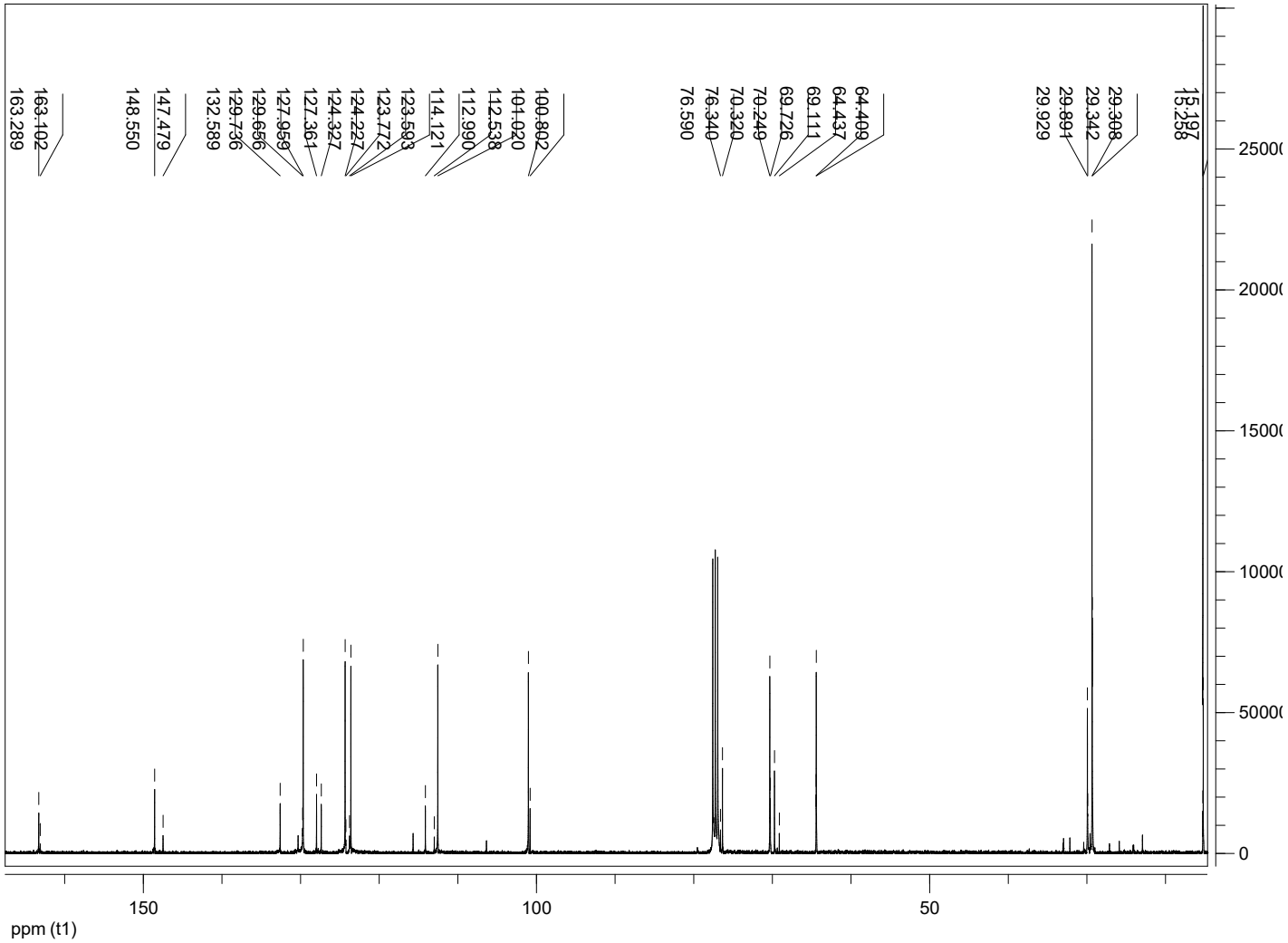
^{1}H NMR spectrum of ***trans*-(±)-9a** in $CDCl_3$





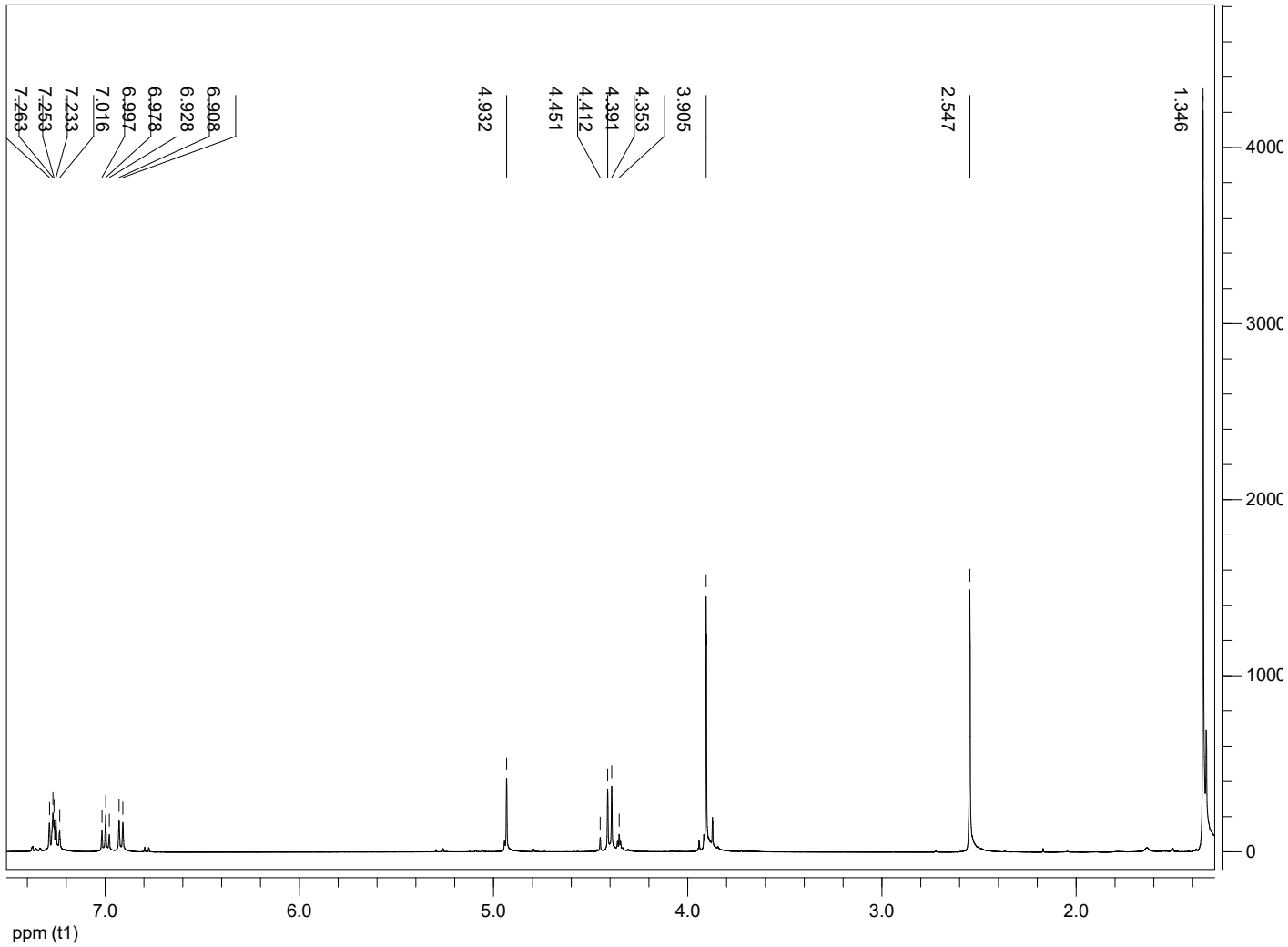
***trans*-(±)-9a**

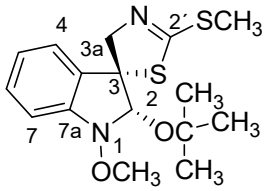
^{13}C NMR spectrum of ***trans*-(±)-9a** in $CDCl_3$



cis-(±)-1-Methoxyspirobrassinol _tert_-butyl ether [_cis_-(±)-9b]

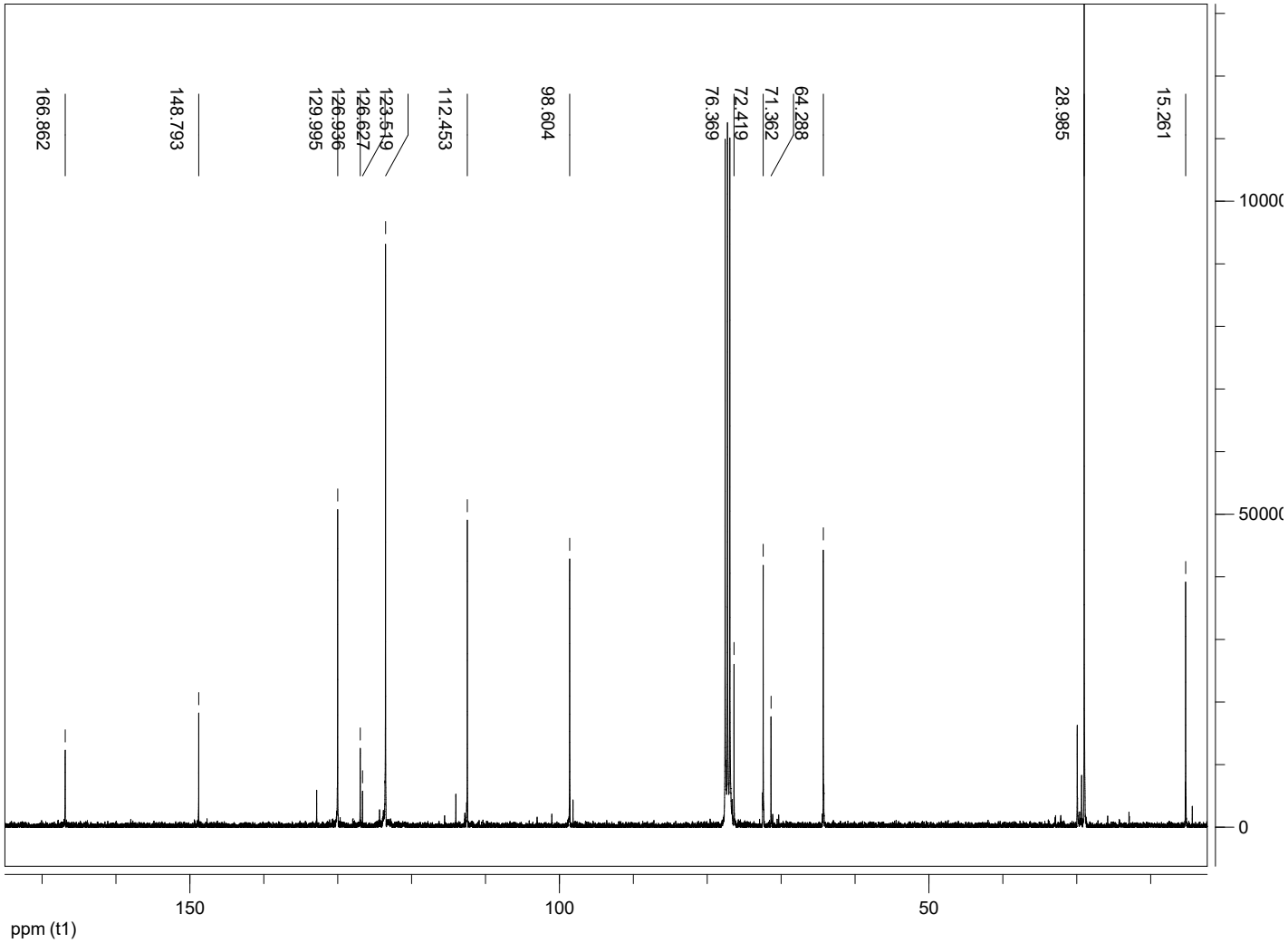
^{1}H NMR spectrum of ***cis*-(±)-9b** in $CDCl_3$





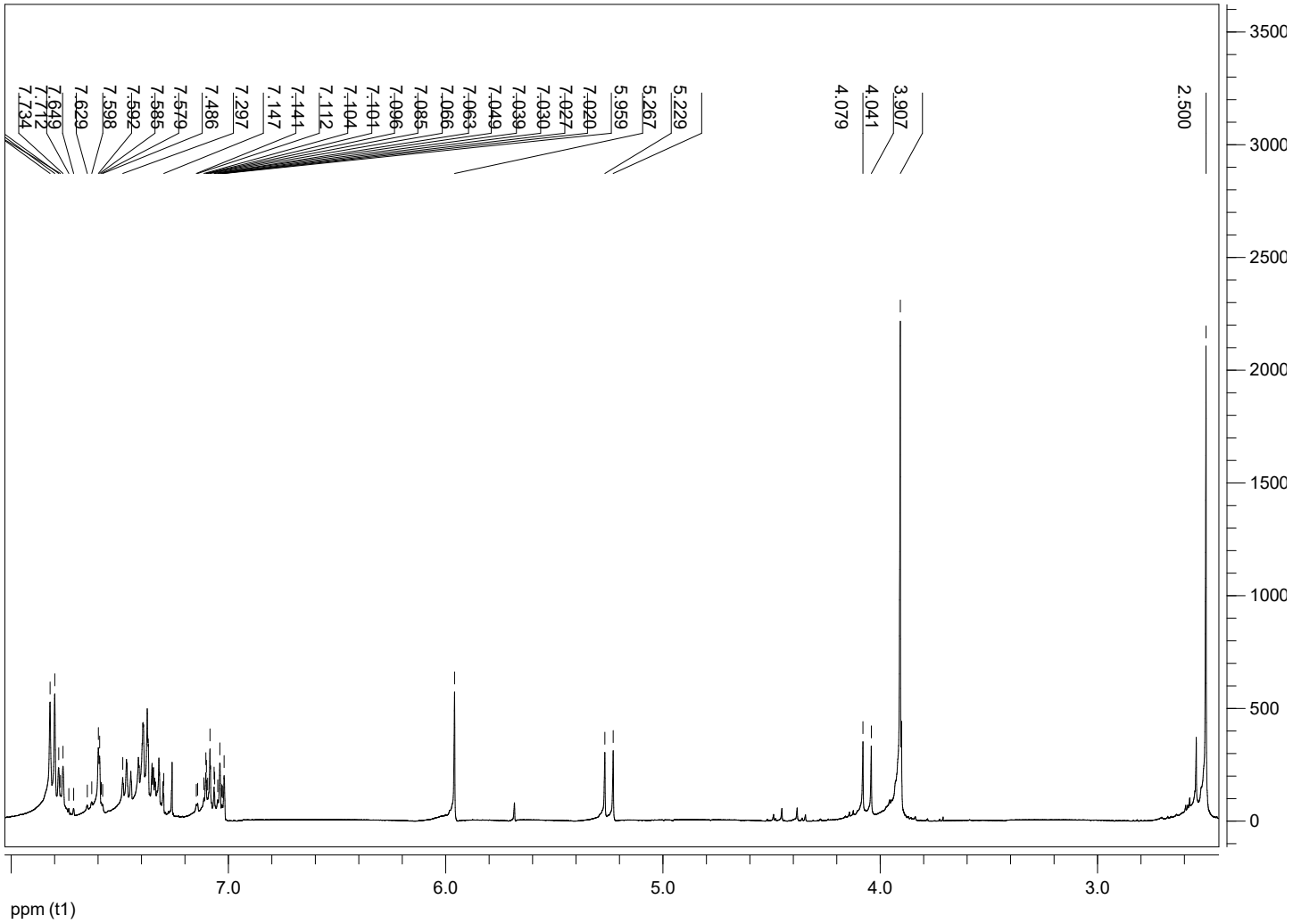
***cis*-(±)-9b**

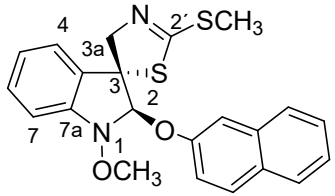
^{13}C NMR spectrum of ***cis*-(±)-9b** in $CDCl_3$



trans-(±)-1-Methoxyspirobrassinol naphth-2-yl ether [_trans_-(±)-11a]

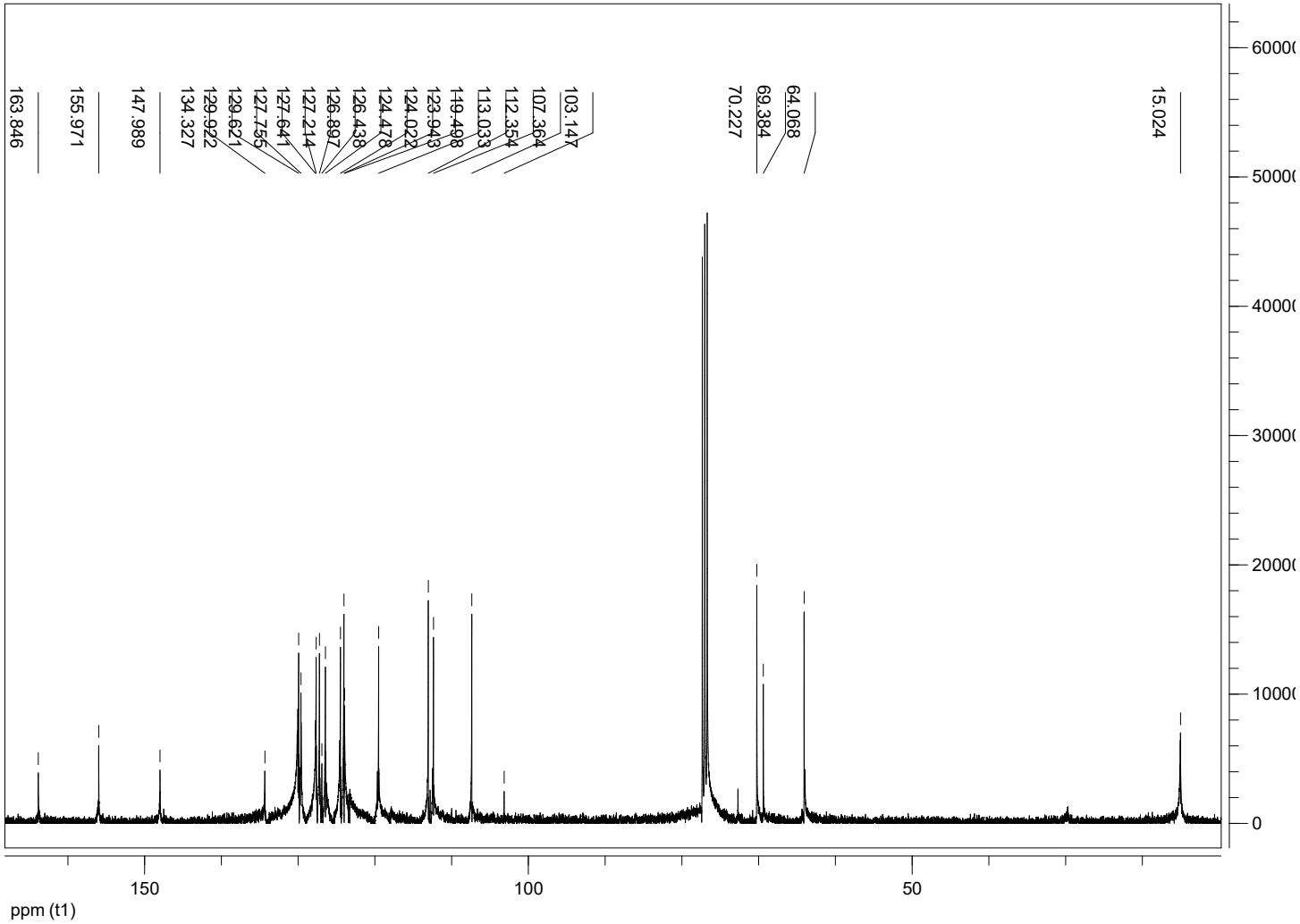
^{1}H NMR spectrum of ***trans*-(±)-11a** in $CDCl_3$





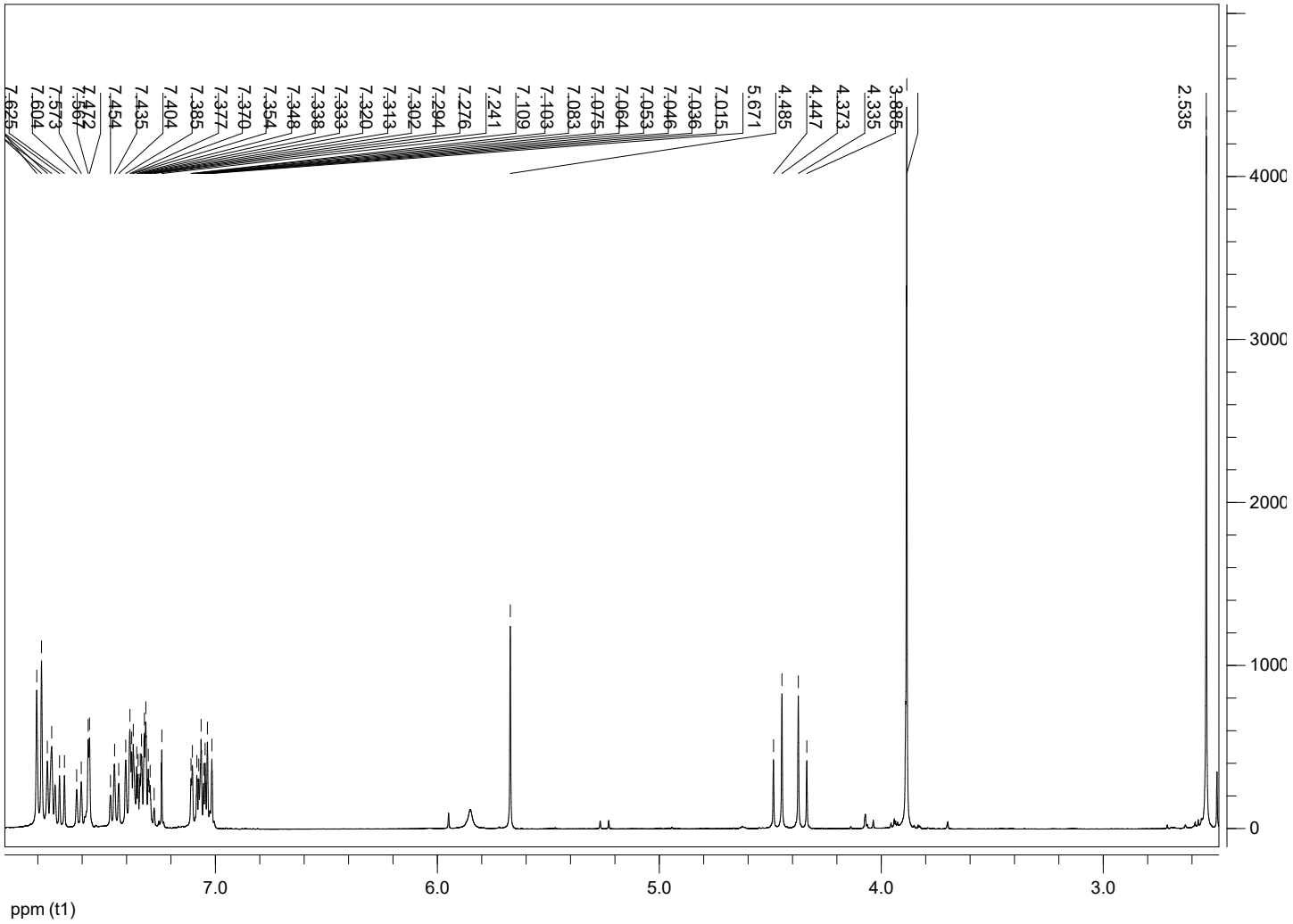
***trans*-(±)-11a**

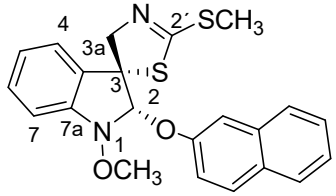
^{13}C NMR spectrum of ***trans*-(±)-11a** in $CDCl_3$



cis-(±)-1-Methoxyspirobrassinol naphth-2-yl ether [_cis_-(±)-11b]

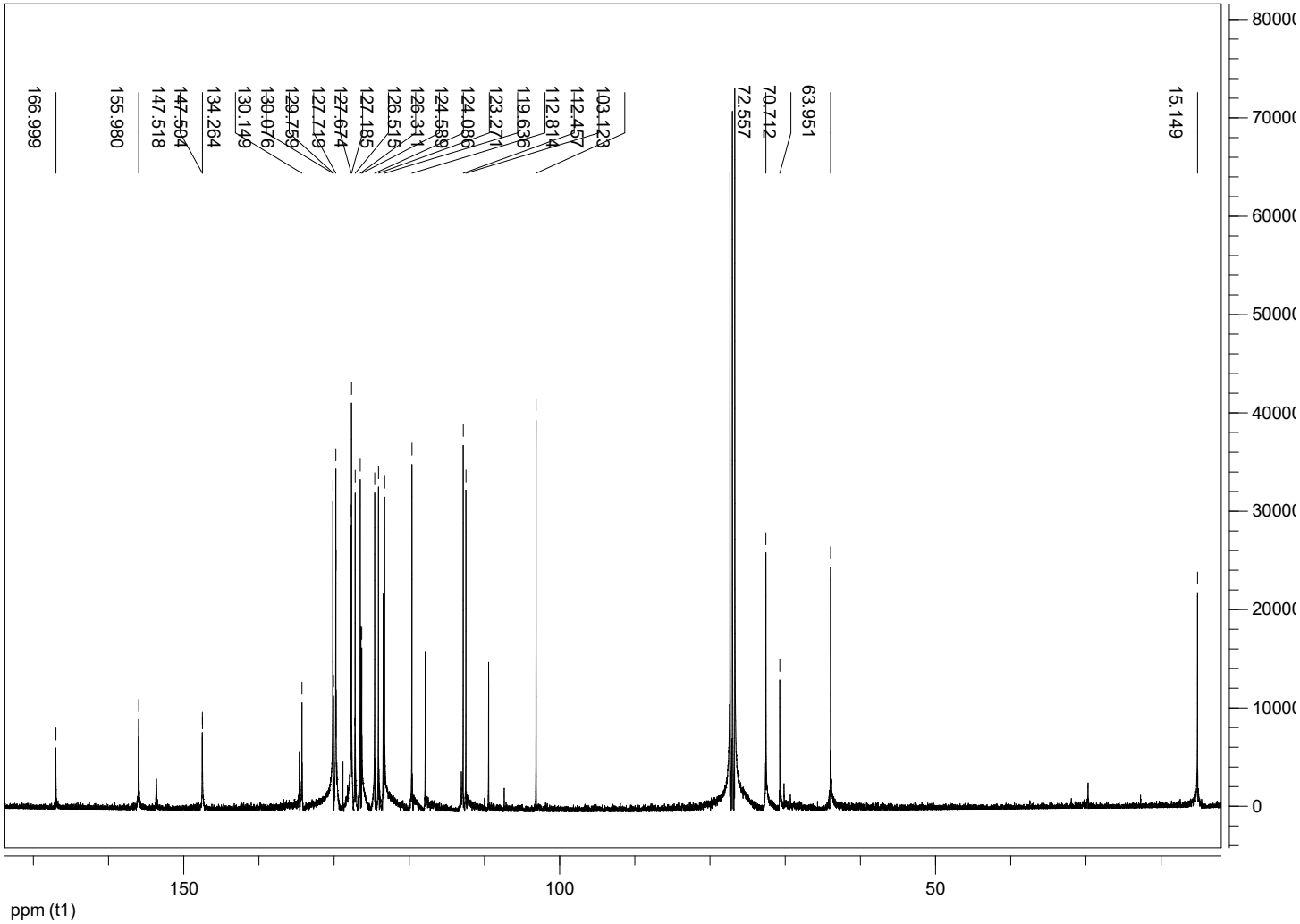
^{1}H NMR spectrum of ***cis*-(±)-11b** in $CDCl_3$





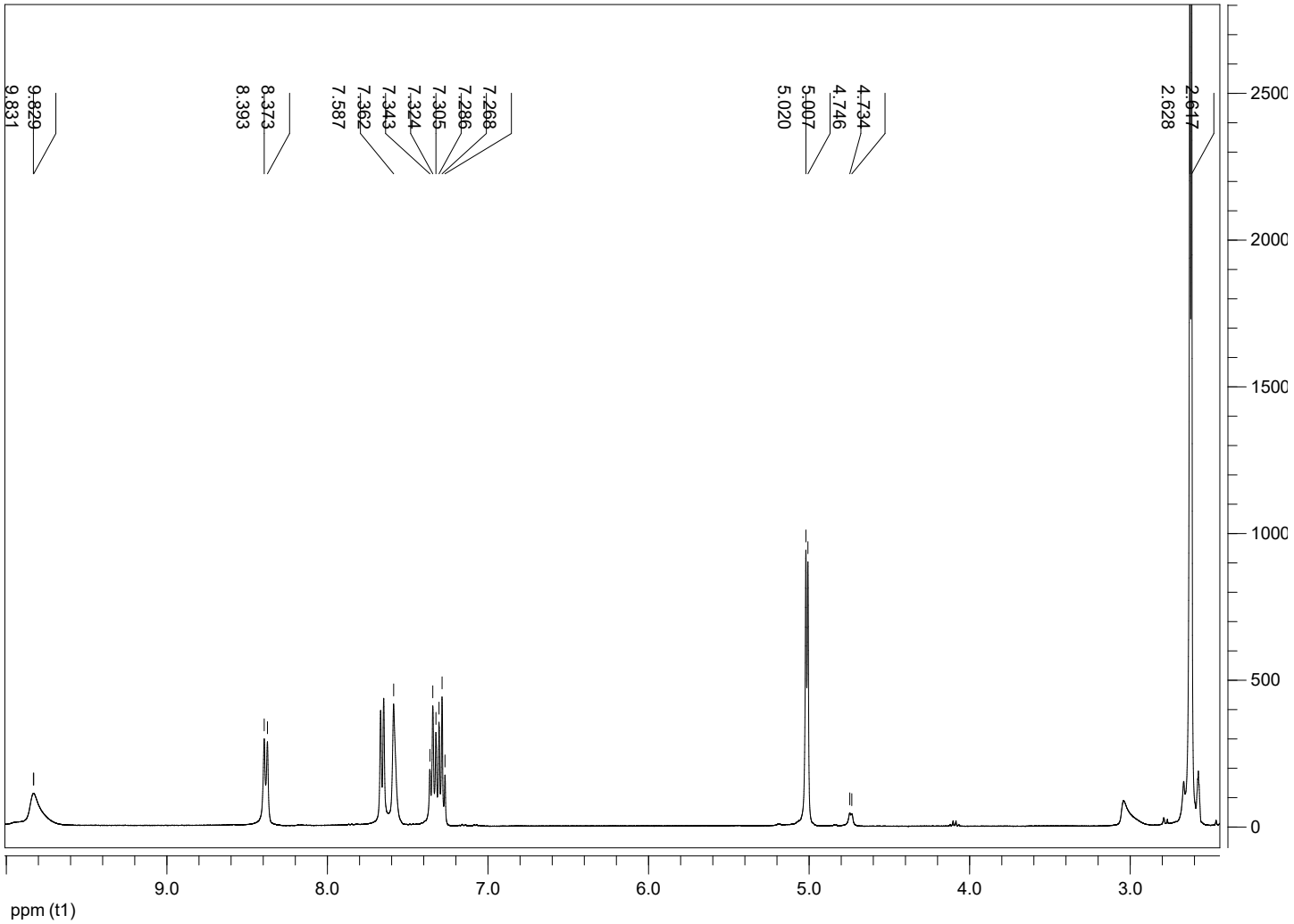
***cis*-(±)-11b**

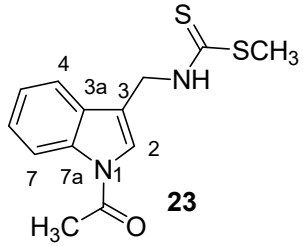
^{13}C NMR spectrum of ***cis*-(±)-11b** in $CDCl_3$



1-Acetylbrassinin (23)

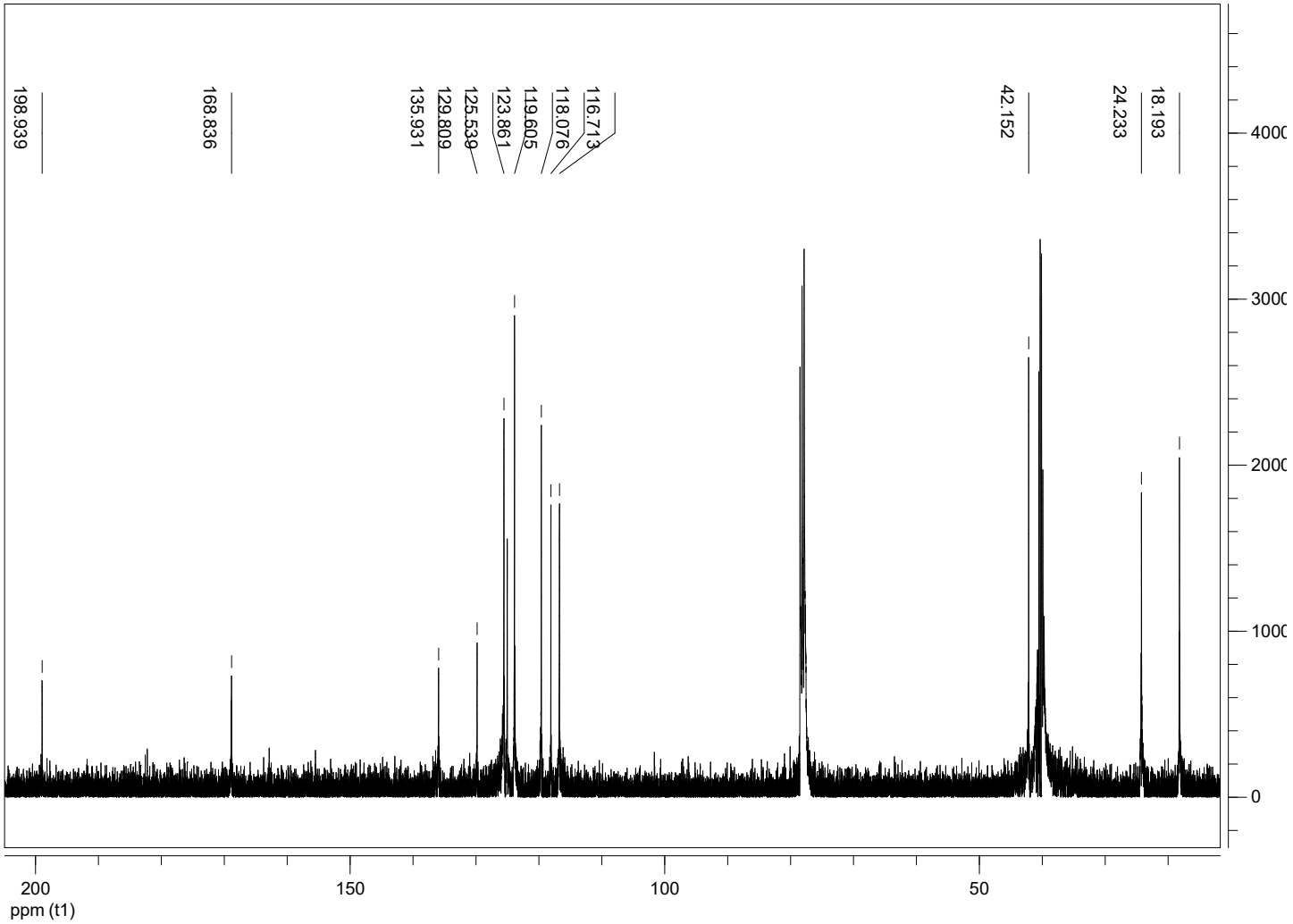
^{1}H NMR spectrum of **23** in DMSO-d_6





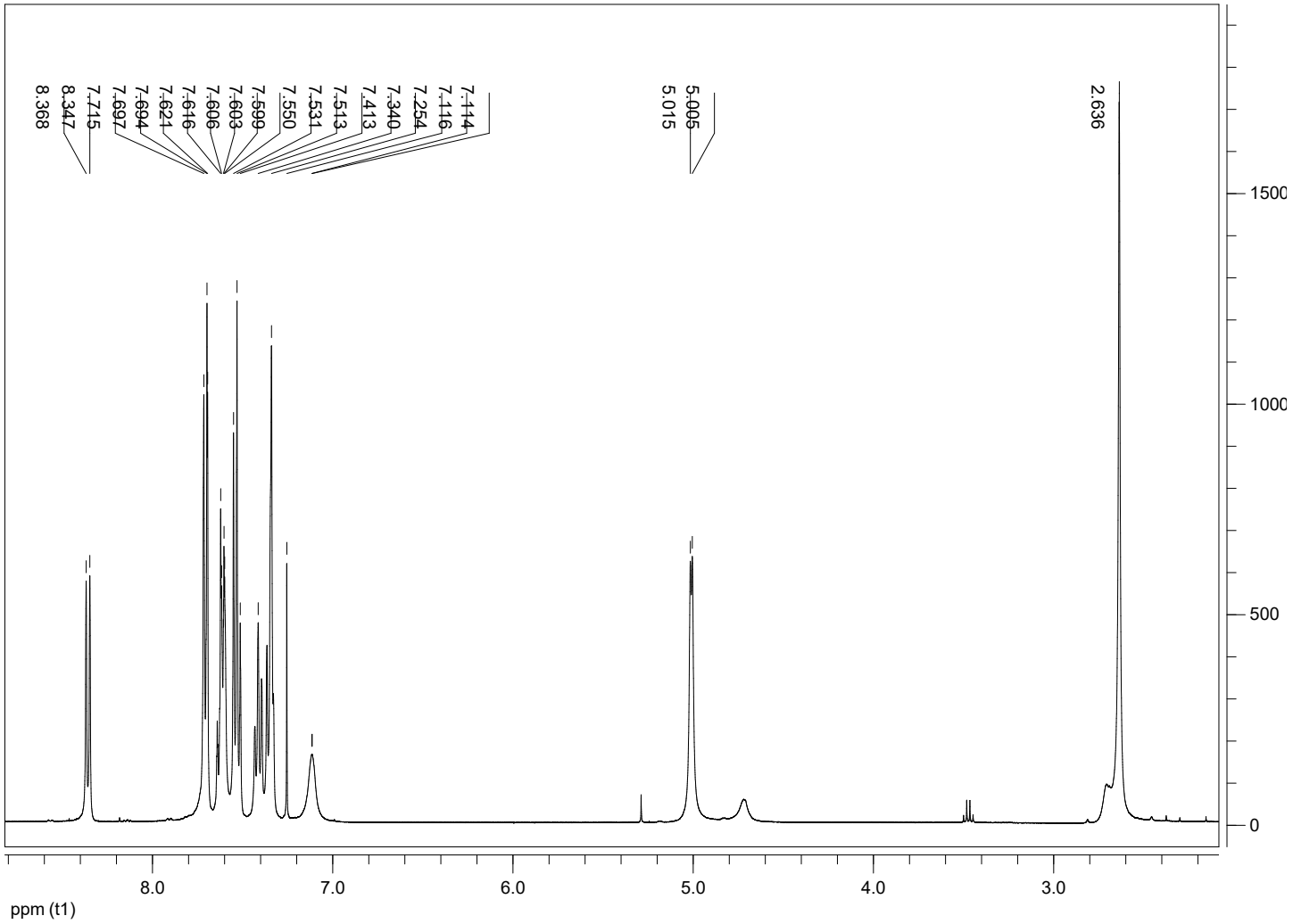
23

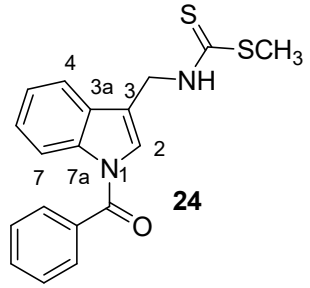
^{13}C NMR spectrum of **23** in DMSO-d_6



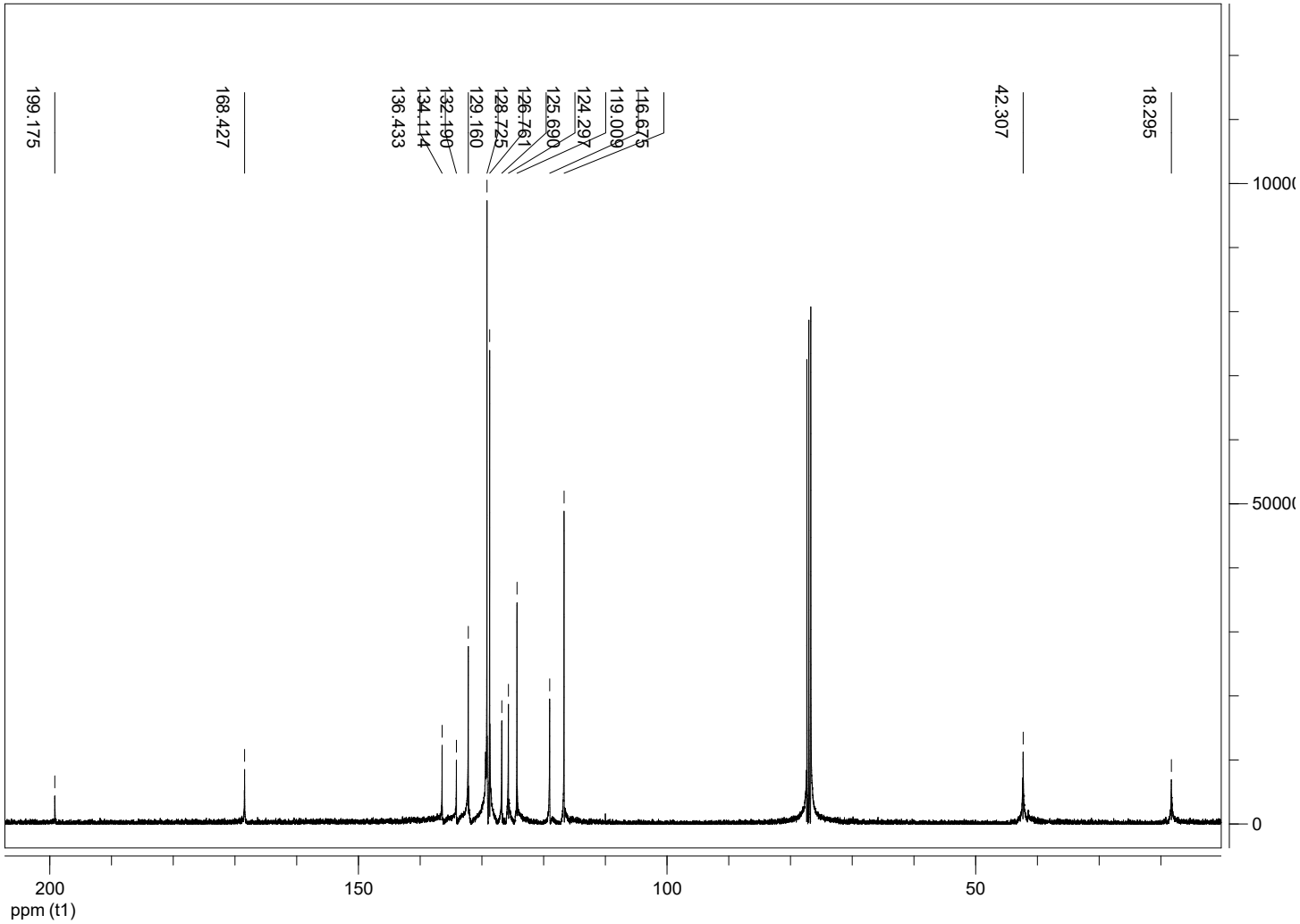
1-Benzoylbrassinin (24)

^{1}H NMR spectrum of **24** in $CDCl_3$



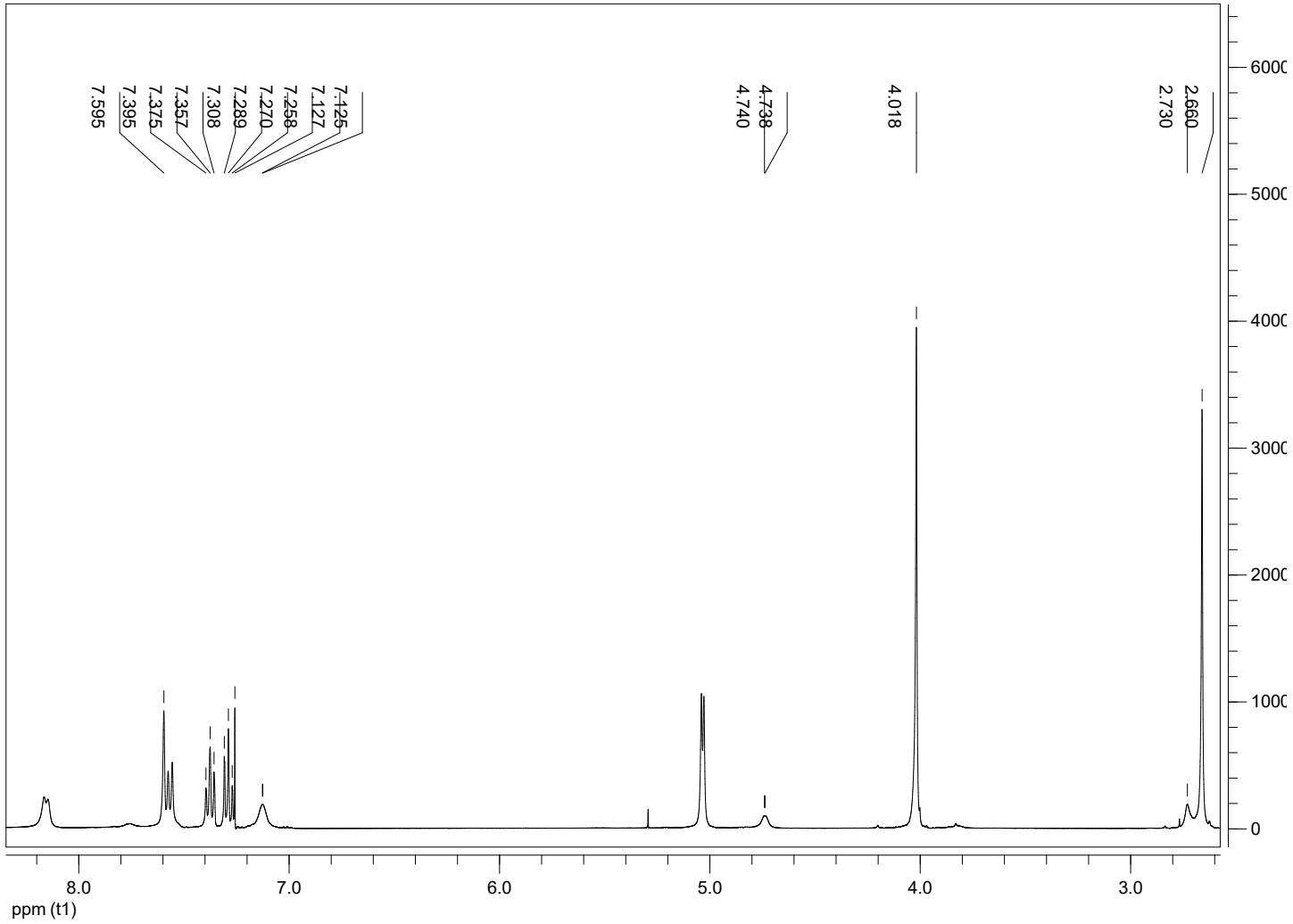


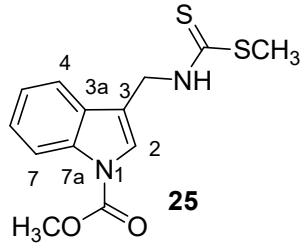
^{13}C NMR spectrum of **24** in $CDCl_3$



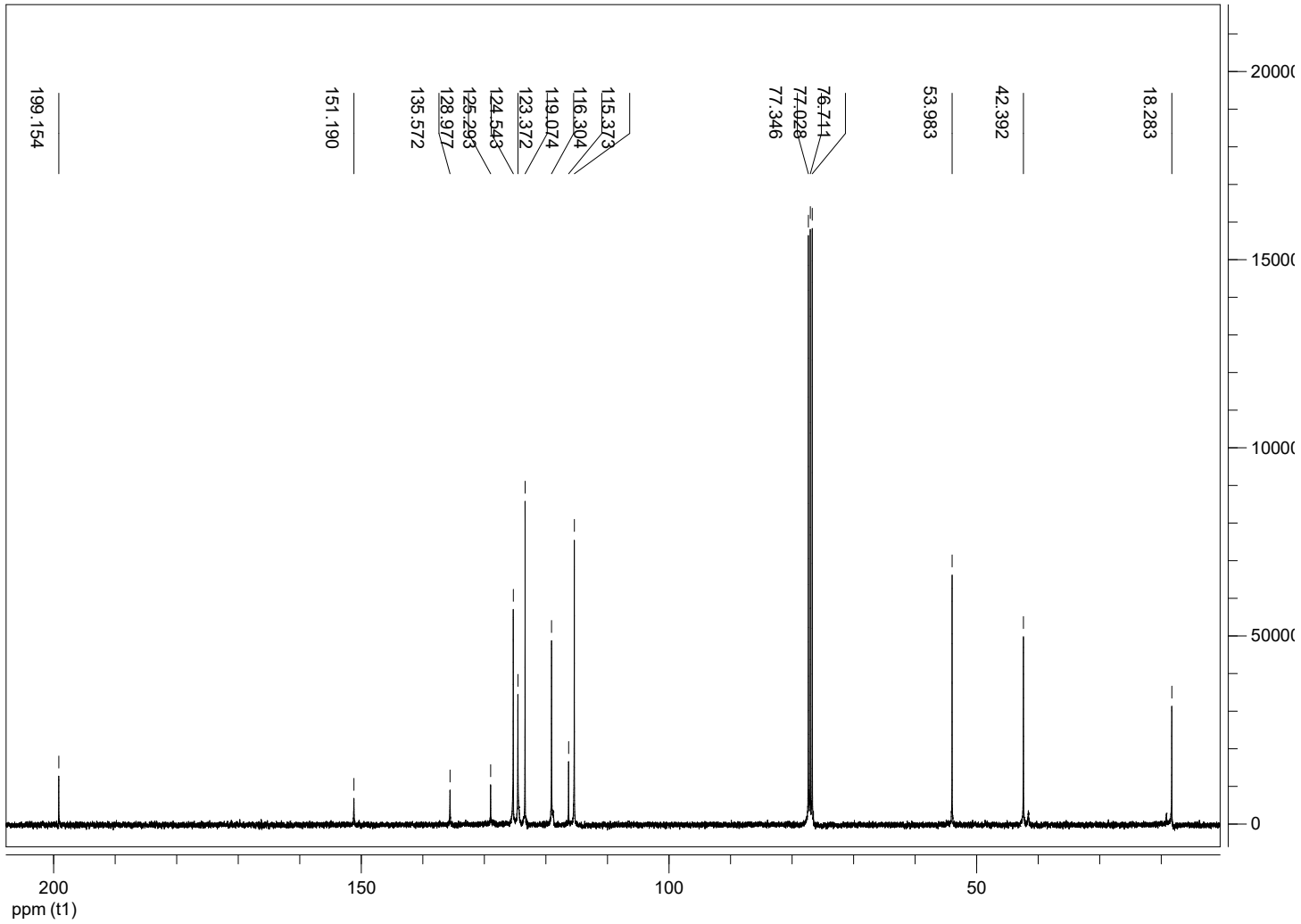
1-(Methoxycarbonyl)brassinin (25)

^{1}H NMR spectrum of **25** in $CDCl_3$



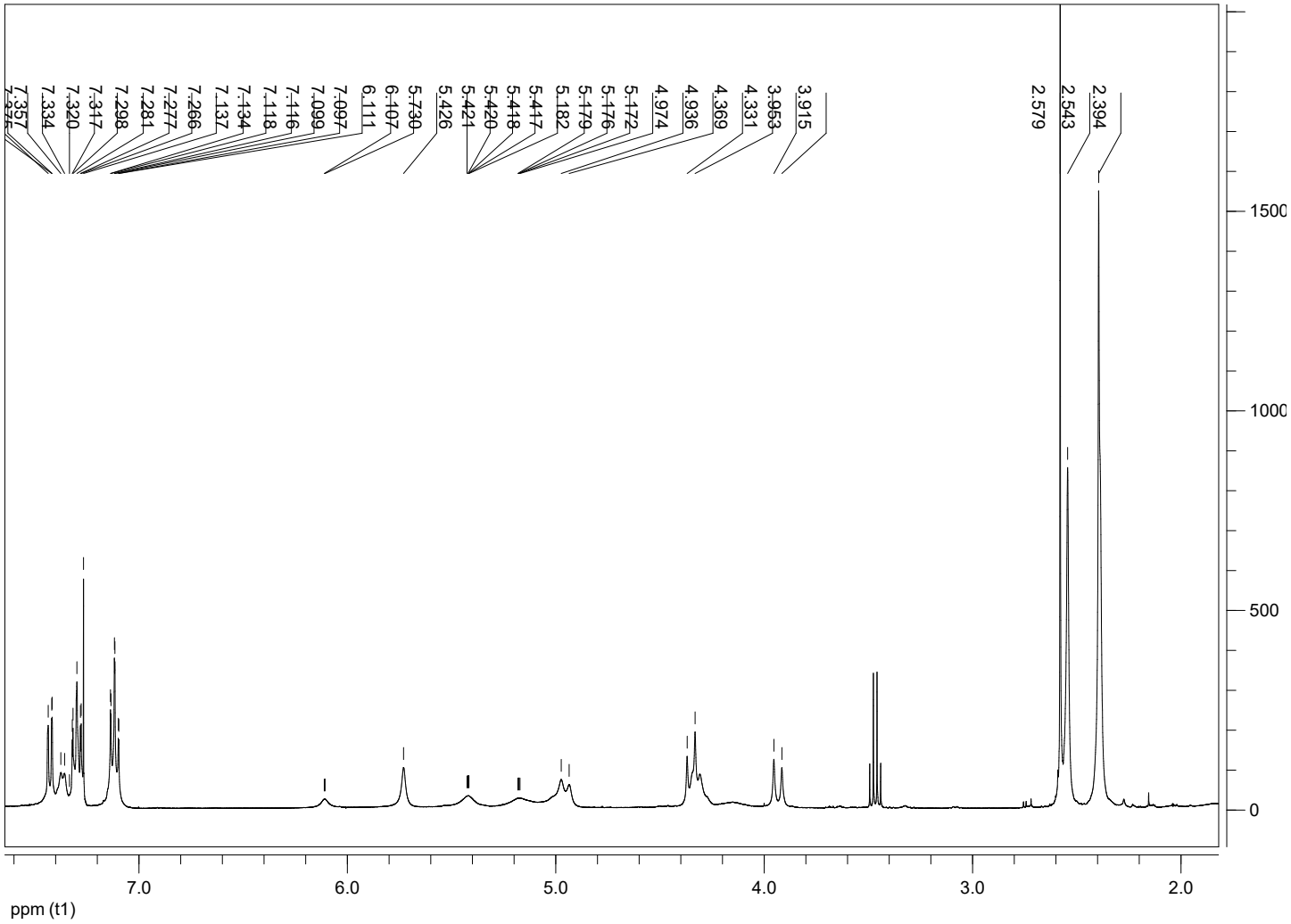


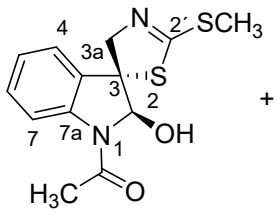
^{13}C NMR spectrum of **25** in $CDCl_3$



trans-(±)- and _cis_-(±)-1-Acetylspirobrassinol [_trans_-(±)-26a and _cis_-(±)-26b]

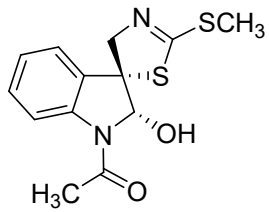
^{1}H NMR spectrum of mixture ***trans*-(±)-26a and *cis*-(±)-26b** in $CDCl_3$





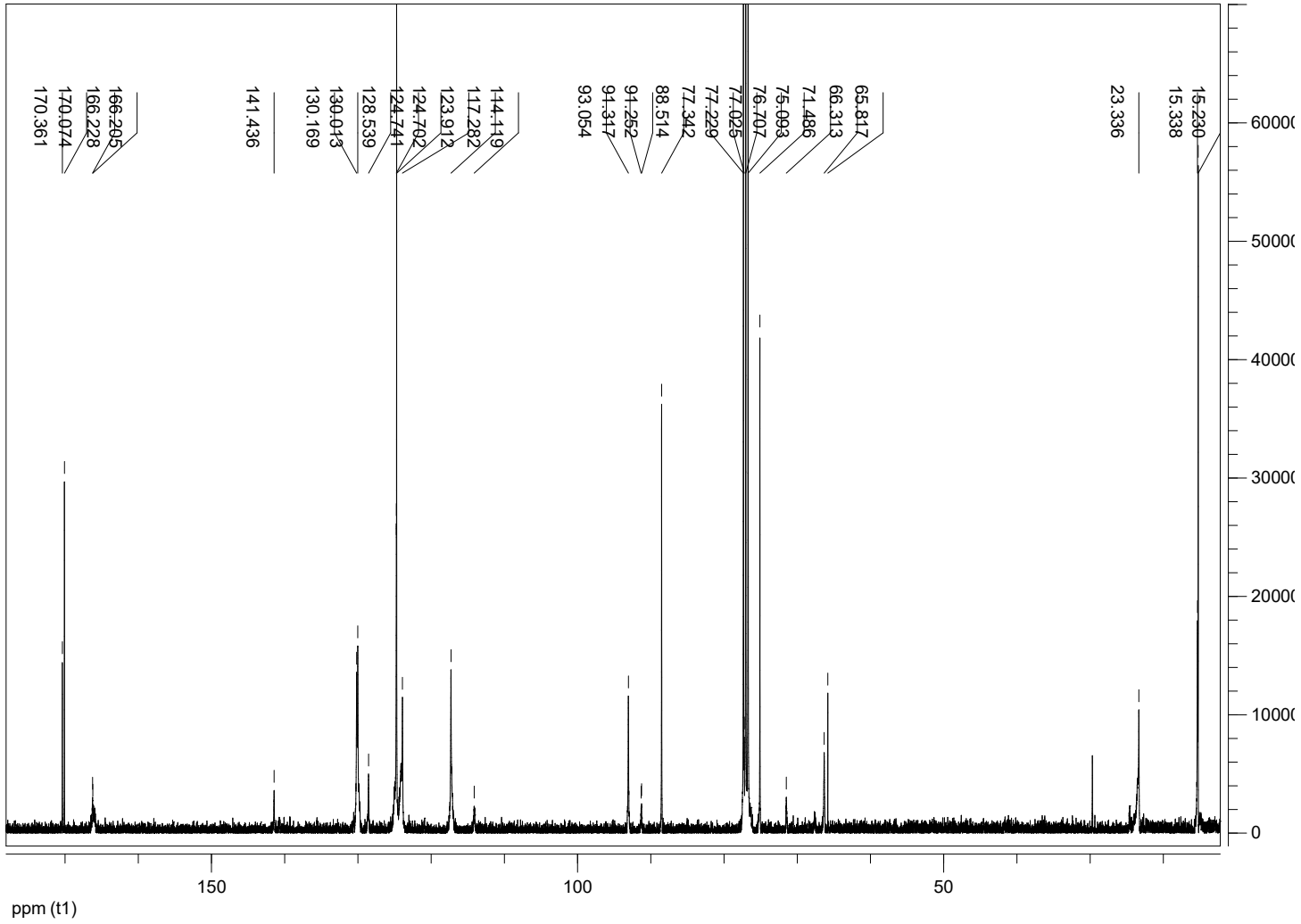
trans-(±)-**26a**

+



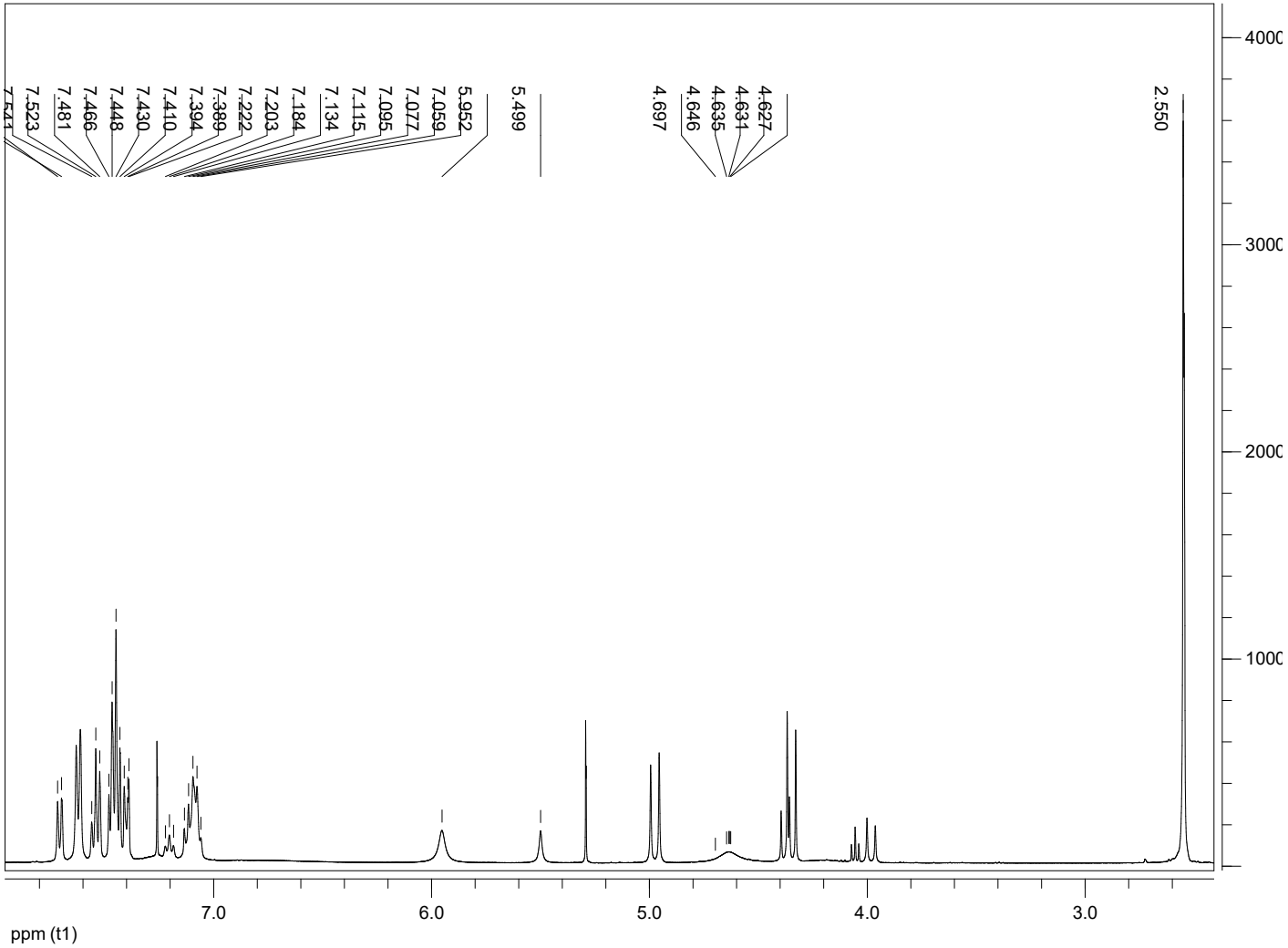
cis-(±)-**26b**

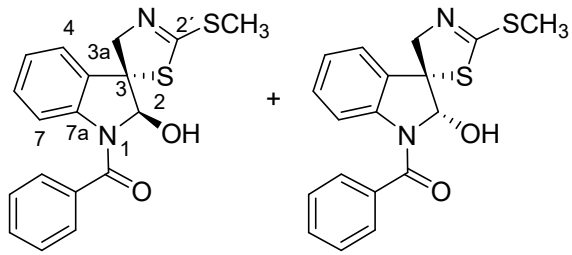
^{13}C NMR spectrum of mixture ***trans*-(±)-26a and *cis*-(±)-26b** in $CDCl_3$



trans-(±)- and _cis_-(±)-1-Benzoylspirobrassinol [_trans_-(±)-27a and _cis_-(±)-27b]

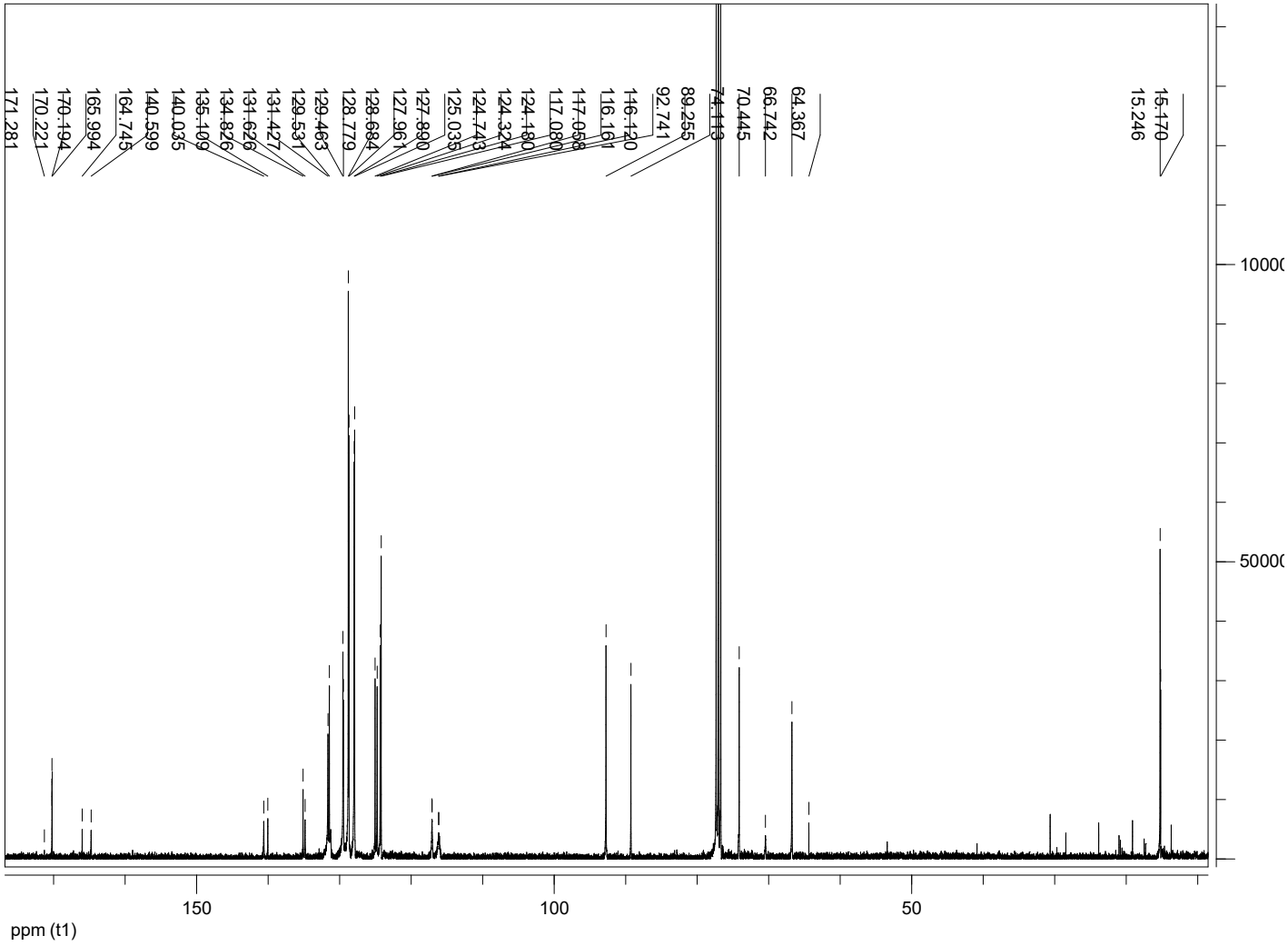
^{1}H NMR spectrum of mixture ***trans*-(±)-27a and *cis*-(±)-27b** in $CDCl_3$





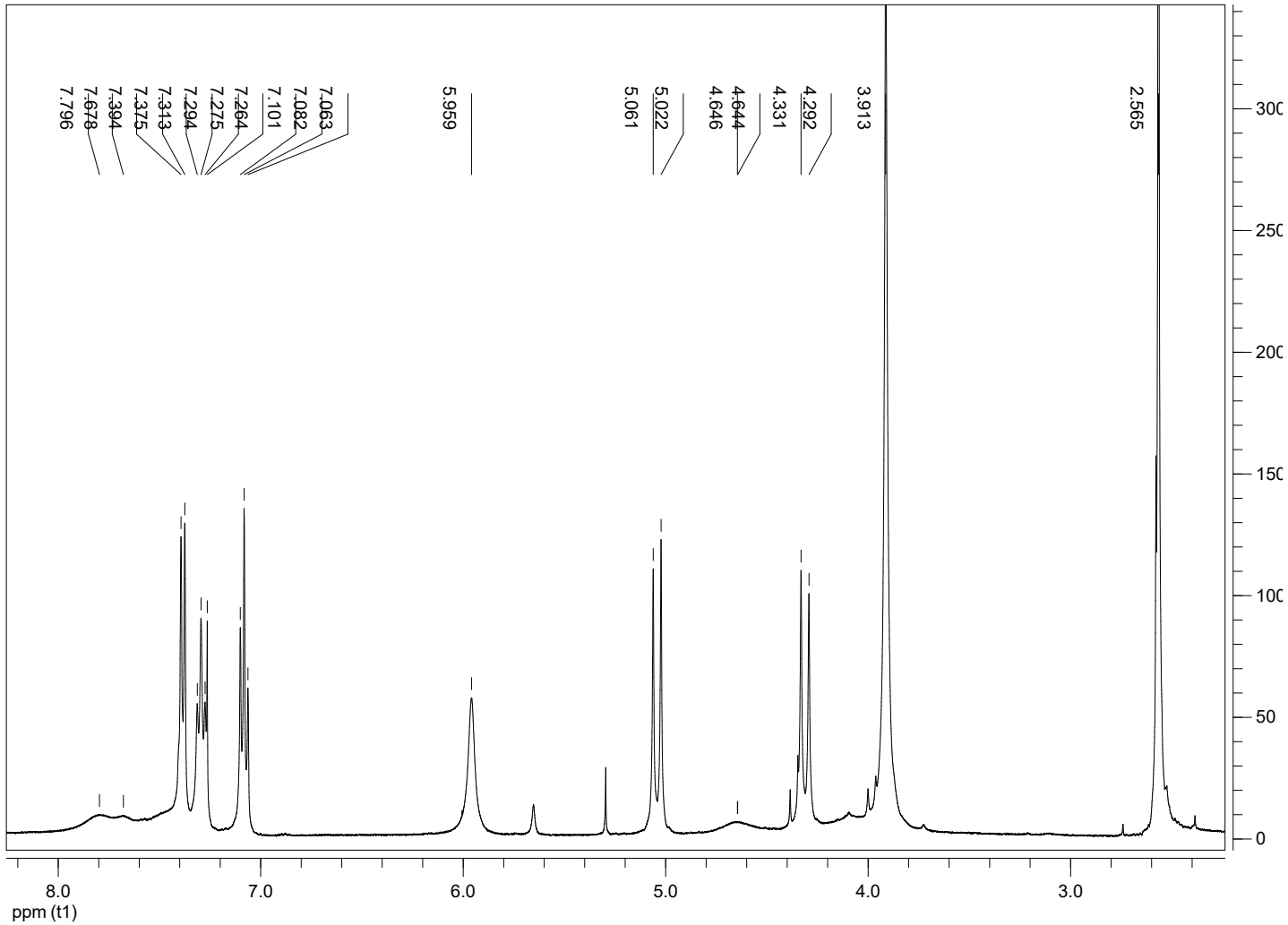
trans-(±)-**27a** *cis*-(±)-**27b**

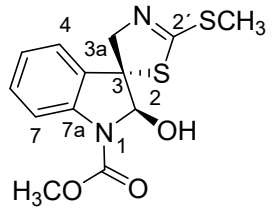
^{13}C NMR spectrum of mixture ***trans*-(±)-27a and *cis*-(±)-27b** in $CDCl_3$



trans-(±)-1-Methoxycarbonylspirobrassinol [_trans_-(±)-28a]

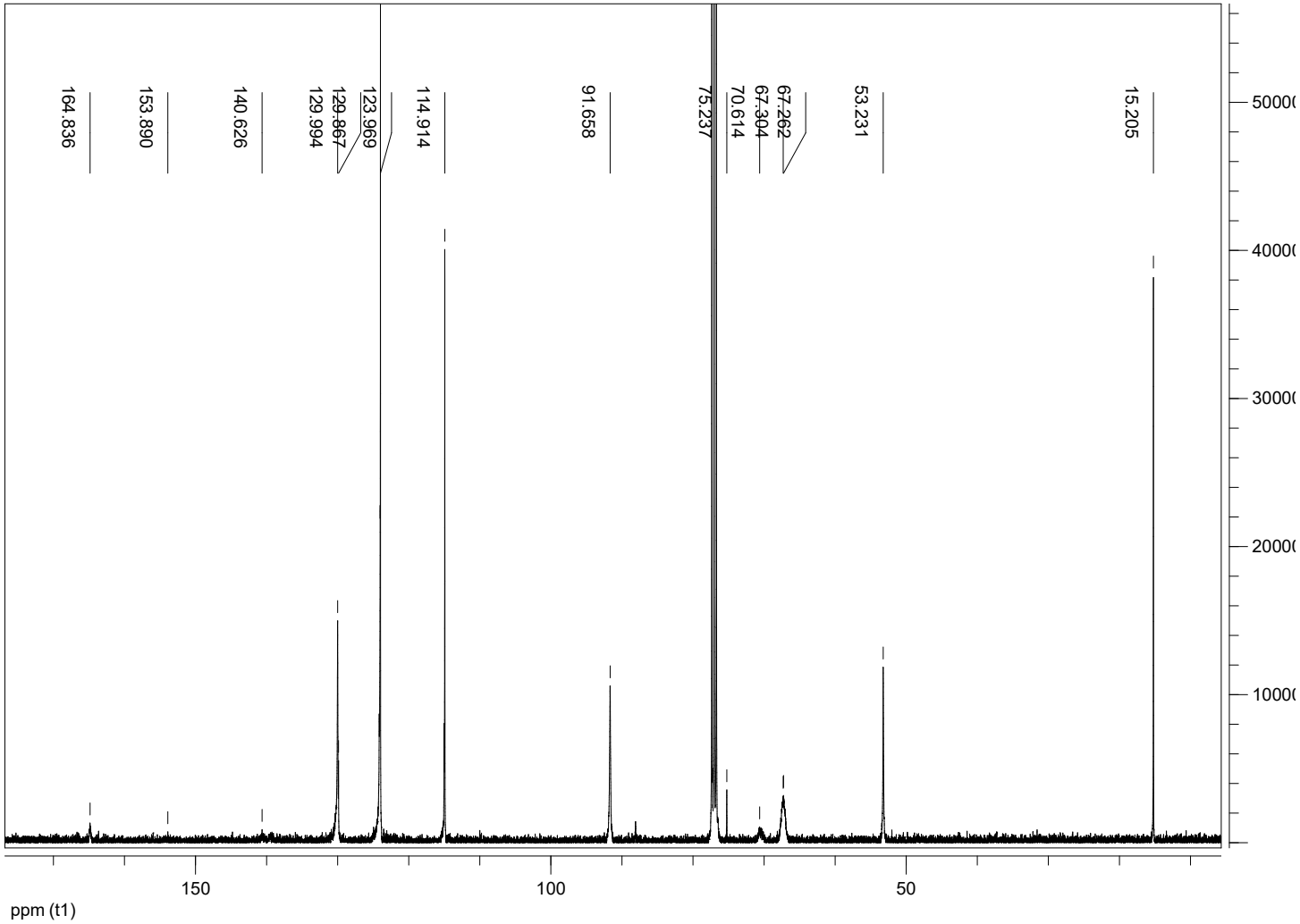
^{1}H NMR spectrum of ***trans*-(±)-28a** in $CDCl_3$





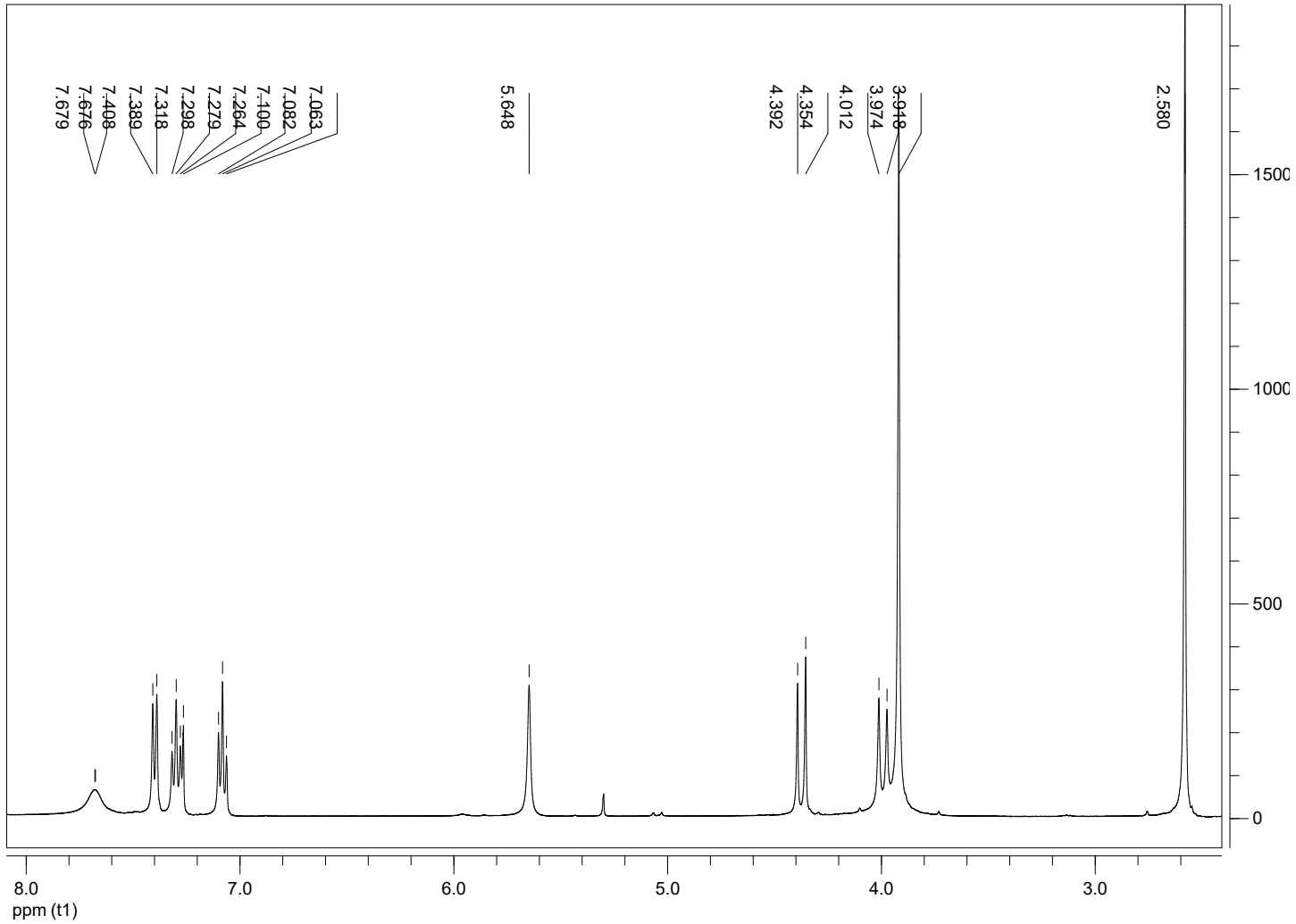
***trans*-(±)-28a**

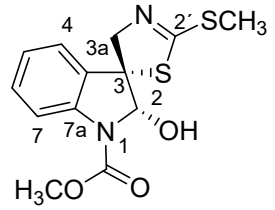
^{13}C NMR spectrum of ***trans*-(±)-28a** in $CDCl_3$



cis-(±)-1-Methoxycarbonylspirobrassinol [_cis_-(±)-28b]

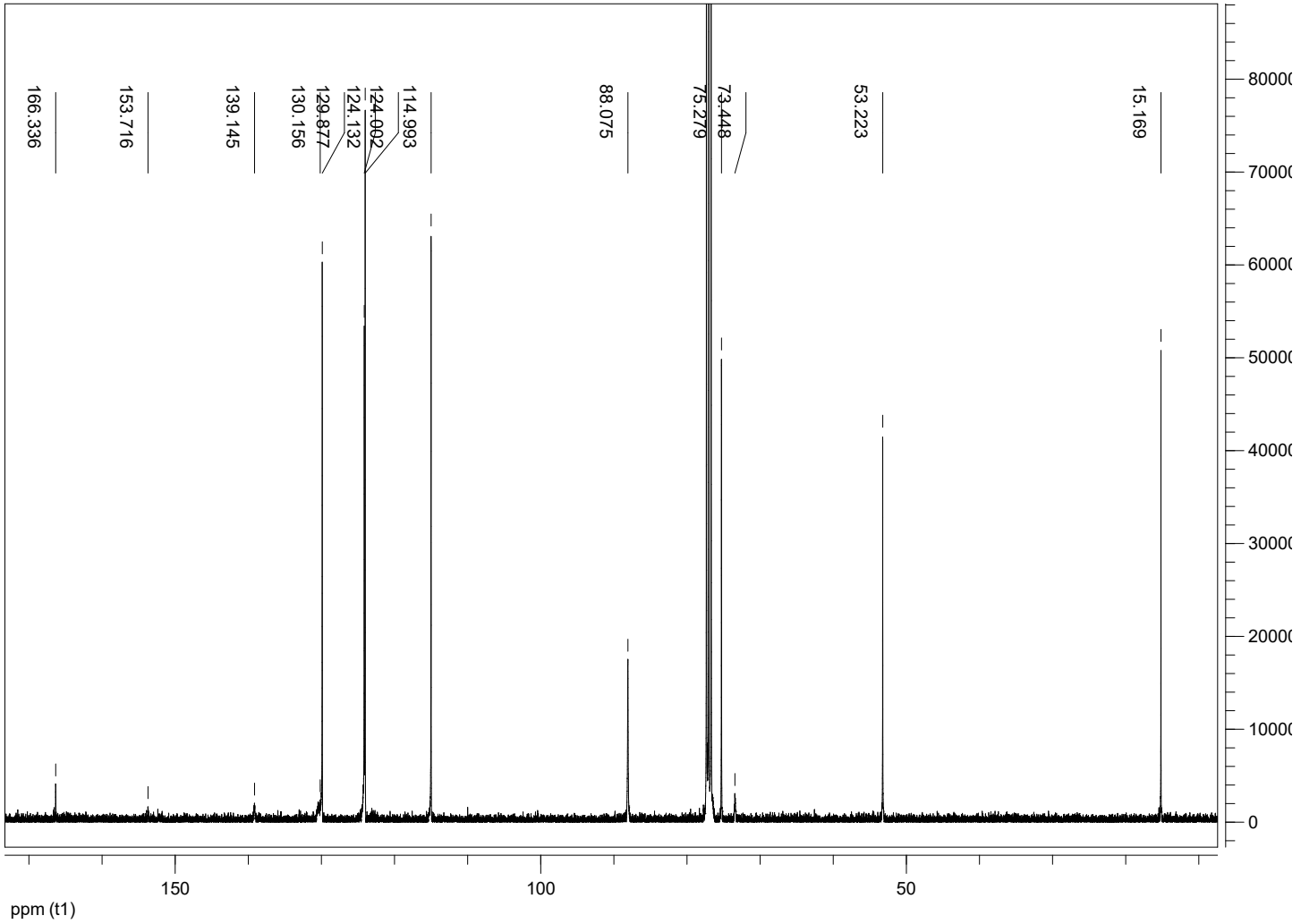
^{1}H NMR spectrum of ***cis*-(±)-28b** in $CDCl_3$



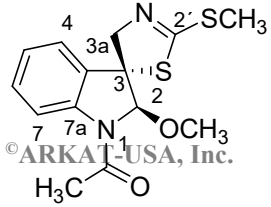


***cis*-(±)-28b**

^{13}C NMR spectrum of ***cis*-(±)-28b** in $CDCl_3$

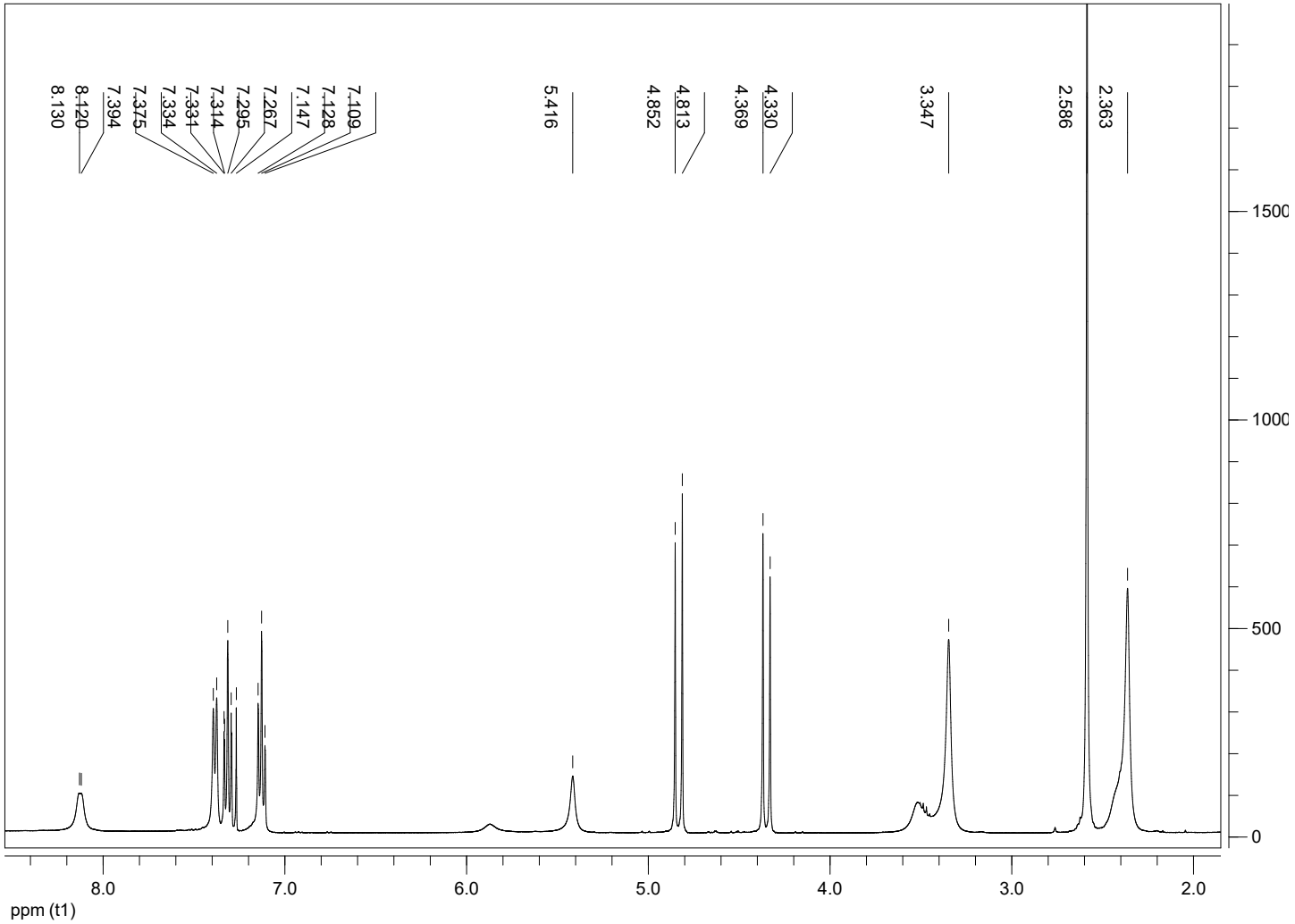


trans-(±)-1-Acetylspirobrassinol methyl ether [_trans_-(±)-30a]

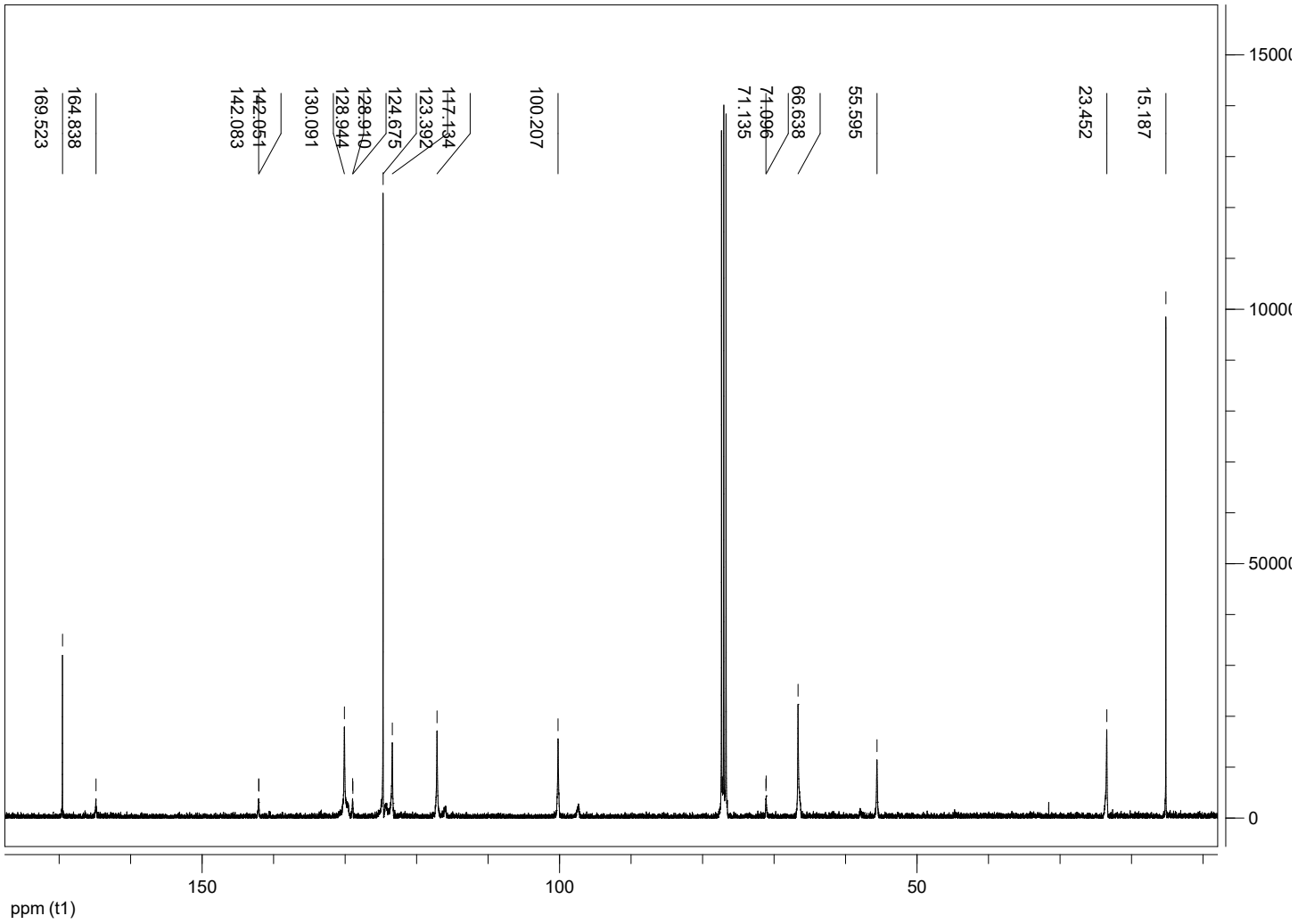


trans-(±)-**30a**

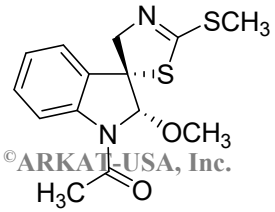
^{1}H NMR spectrum of ***trans*-(±)-30a** in $CDCl_3$



^{13}C NMR spectrum of ***trans*-(±)-30a** in $CDCl_3$

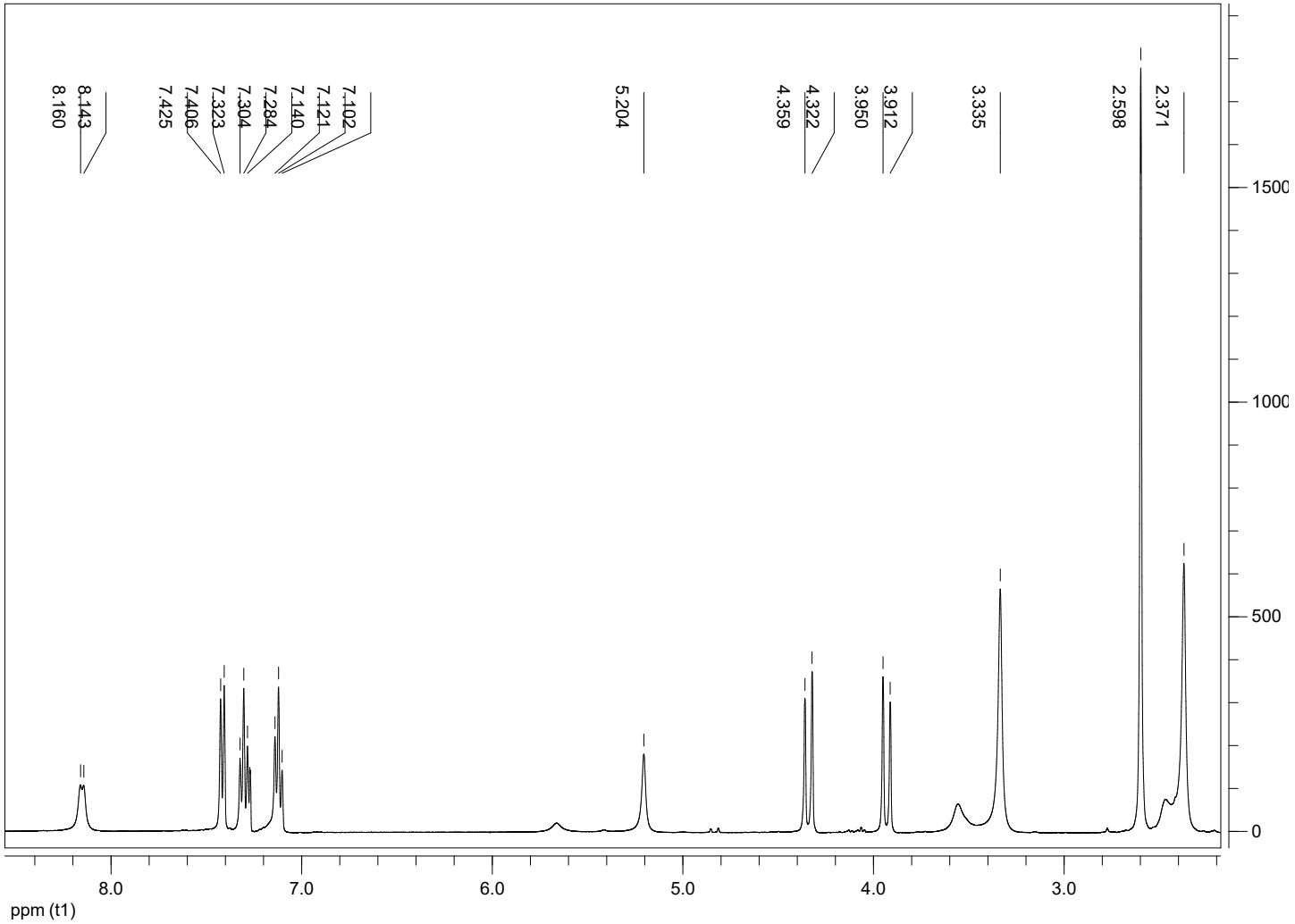


cis-(±)-1-Acetylspirobrasinol methyl ether [(±)-30b]

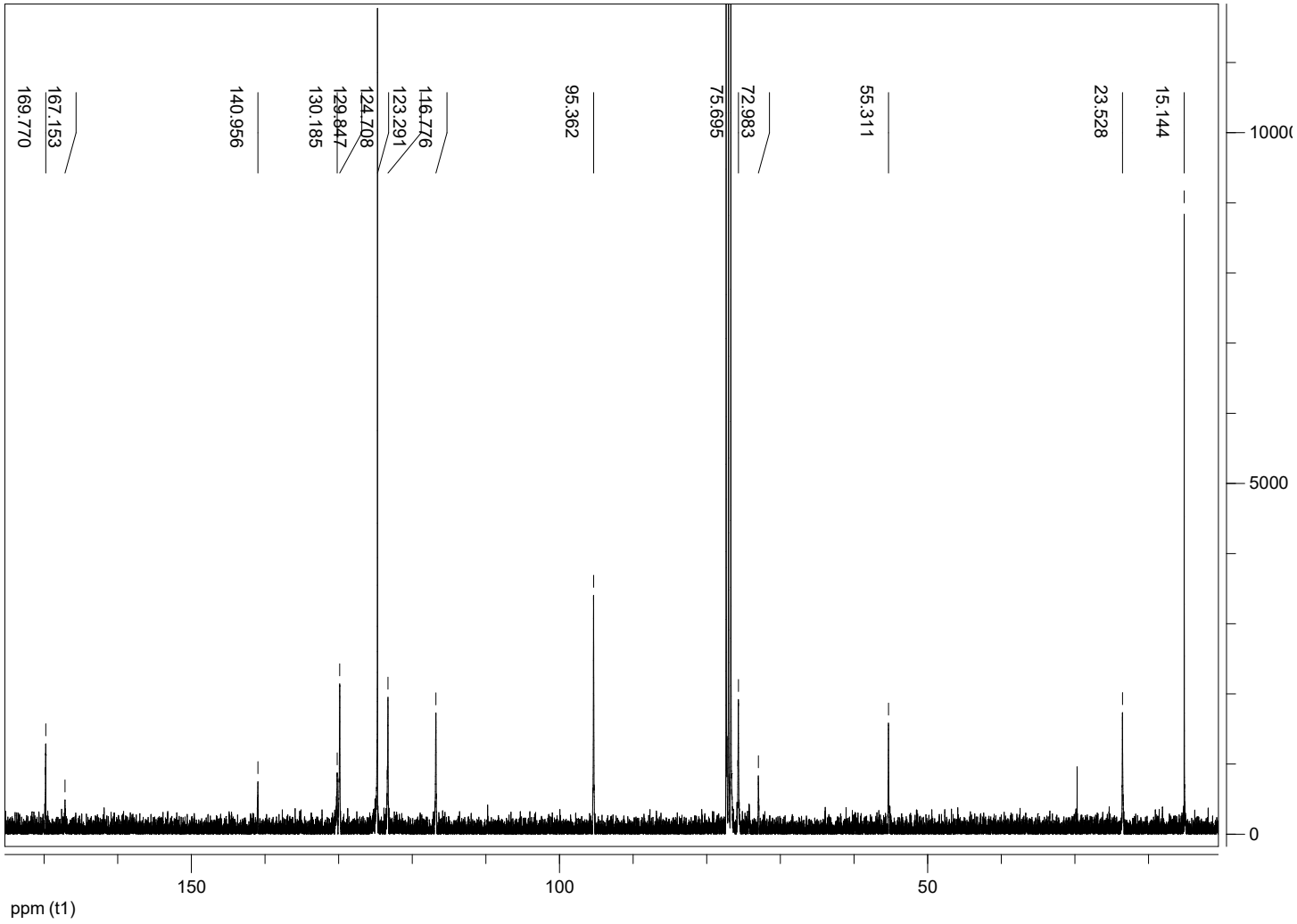


cis-(±)-**30b**

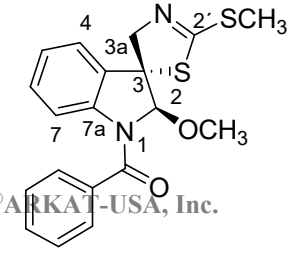
^{1}H NMR spectrum of ***cis*-(±)-30b** in $CDCl_3$



^{13}C NMR spectrum of ***cis*-(±)-30b** in $CDCl_3$

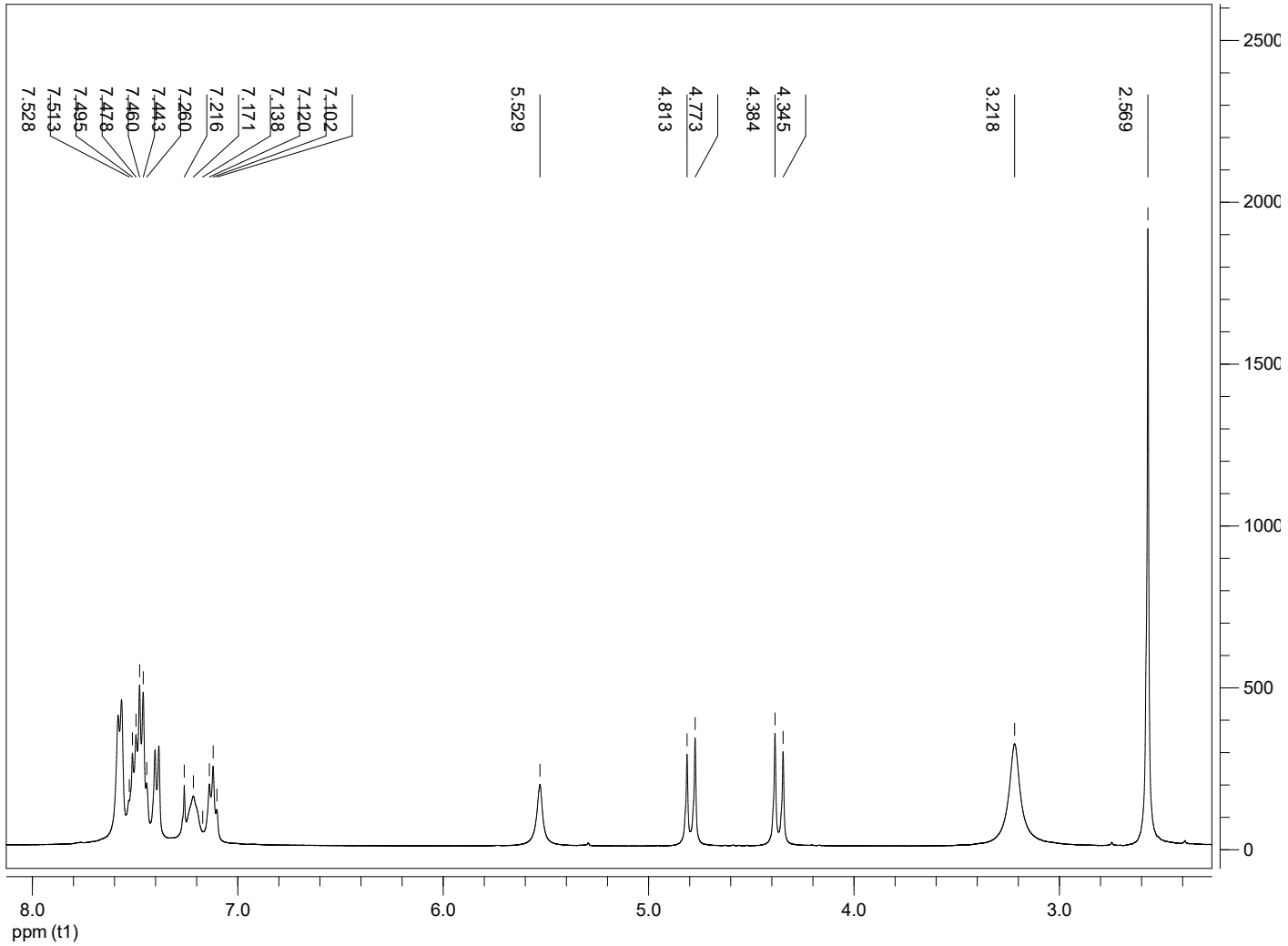


trans-(±)-1-Benzoylspirobrasinol methyl ether [(±)-31a]

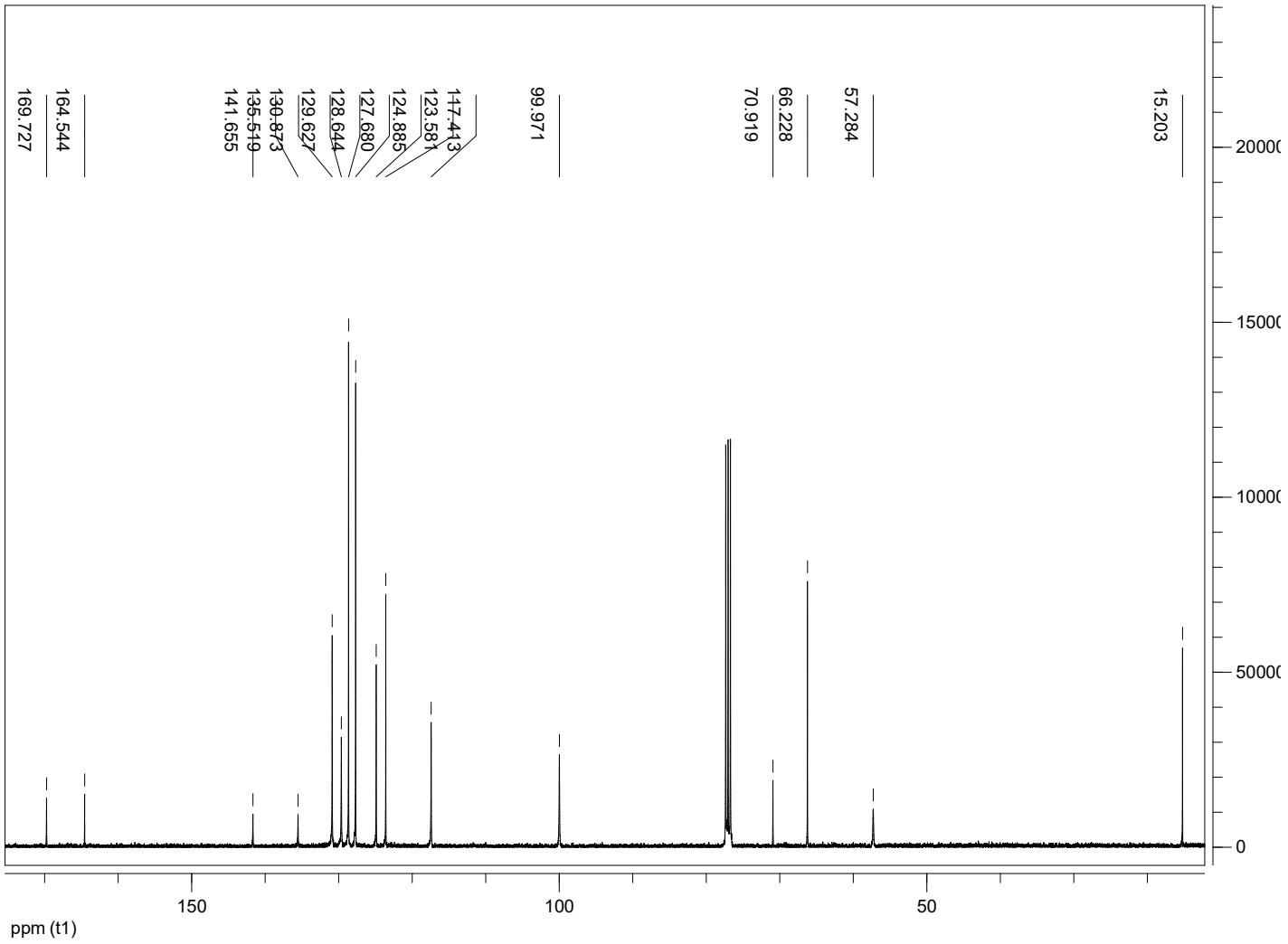


trans-(±)-**31a**

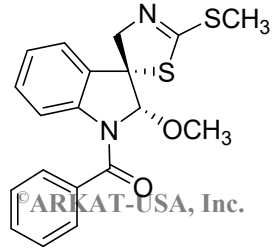
^{1}H NMR spectrum of ***trans*-(±)-31a** in $CDCl_3$



^{13}C NMR spectrum of ***trans*-(±)-31a** in $CDCl_3$

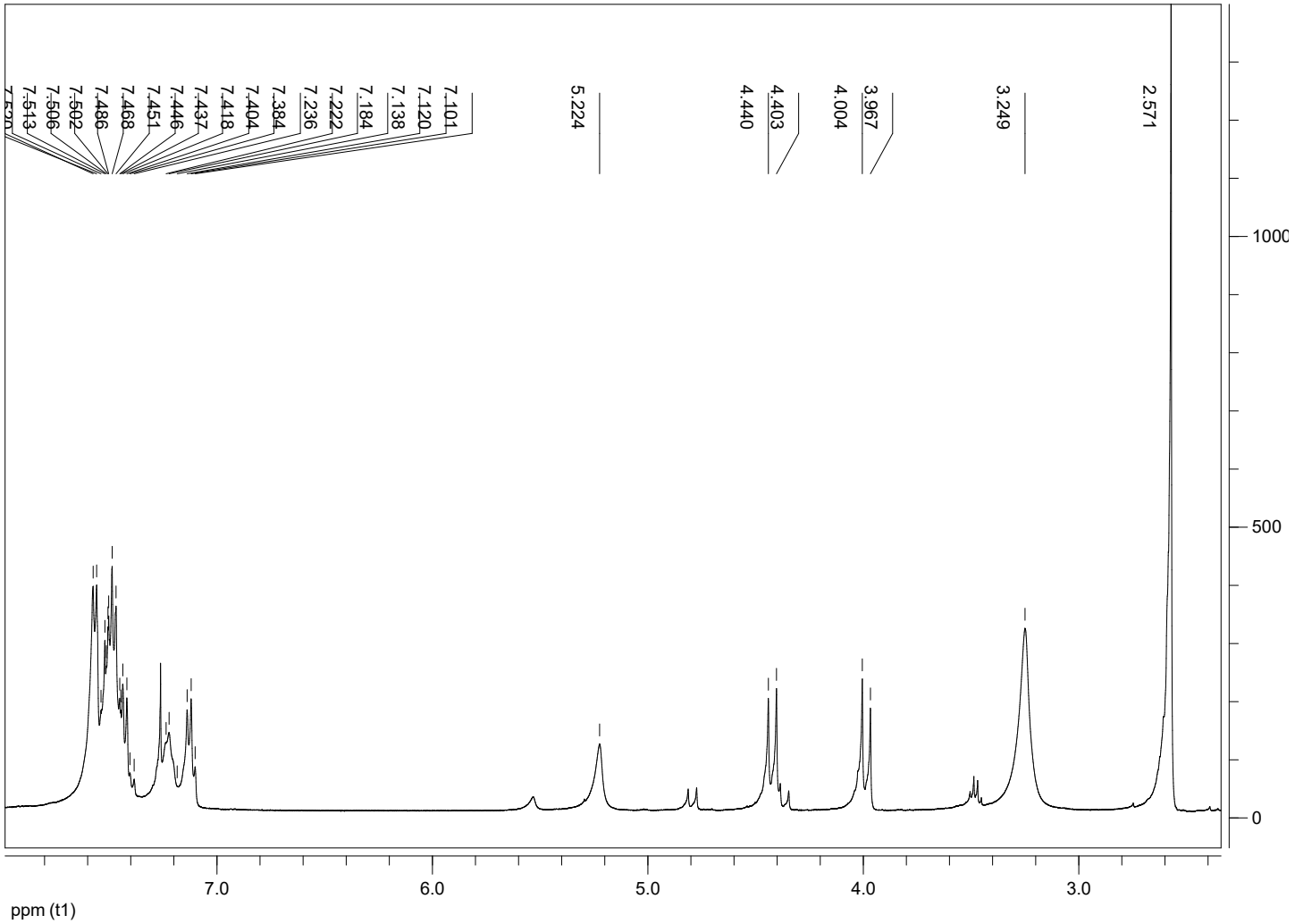


cis-(±)-1-Benzoylspirobrasinol methyl ether [(±)-31b]

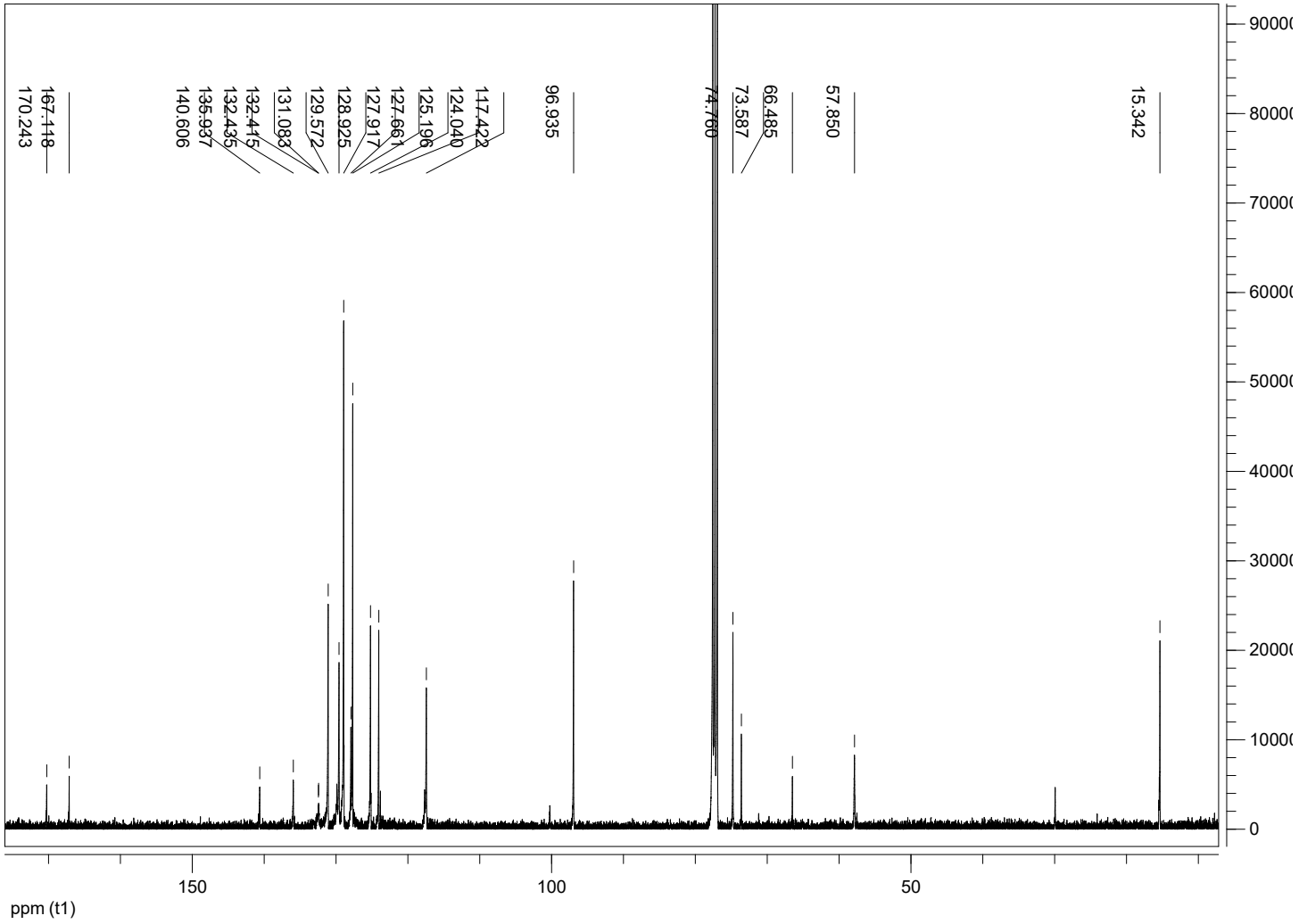


cis-(±)-**31b**

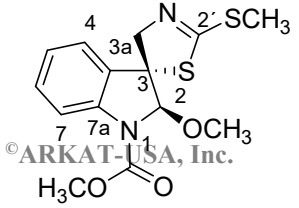
^{1}H NMR spectrum of ***cis*-(±)-31b** in $CDCl_3$



^{13}C NMR spectrum of ***cis*-(±)-31b** in $CDCl_3$

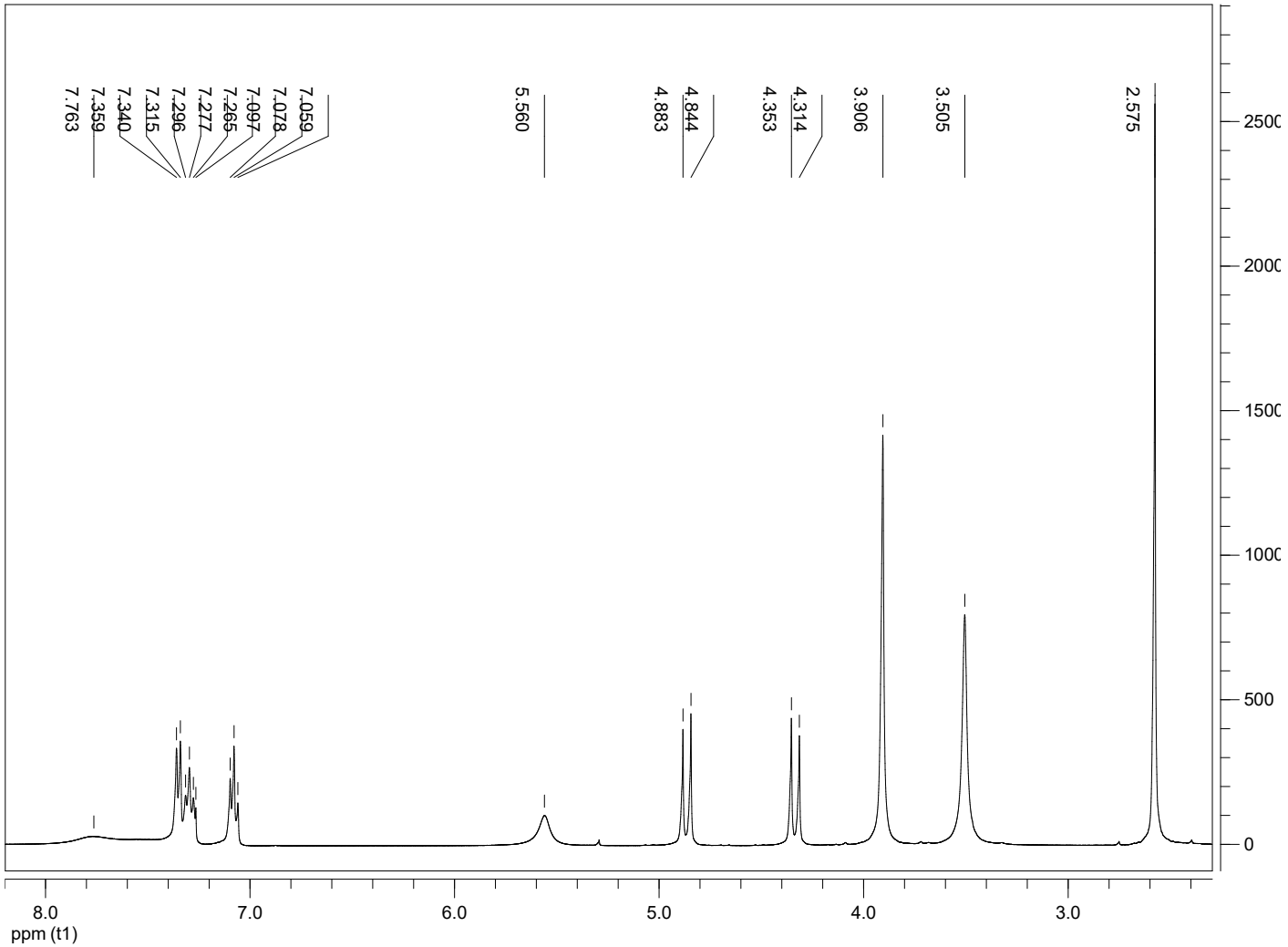


trans-(±)-1-Methoxycarbonylspirobrasinol methyl ether [(±)-32a]

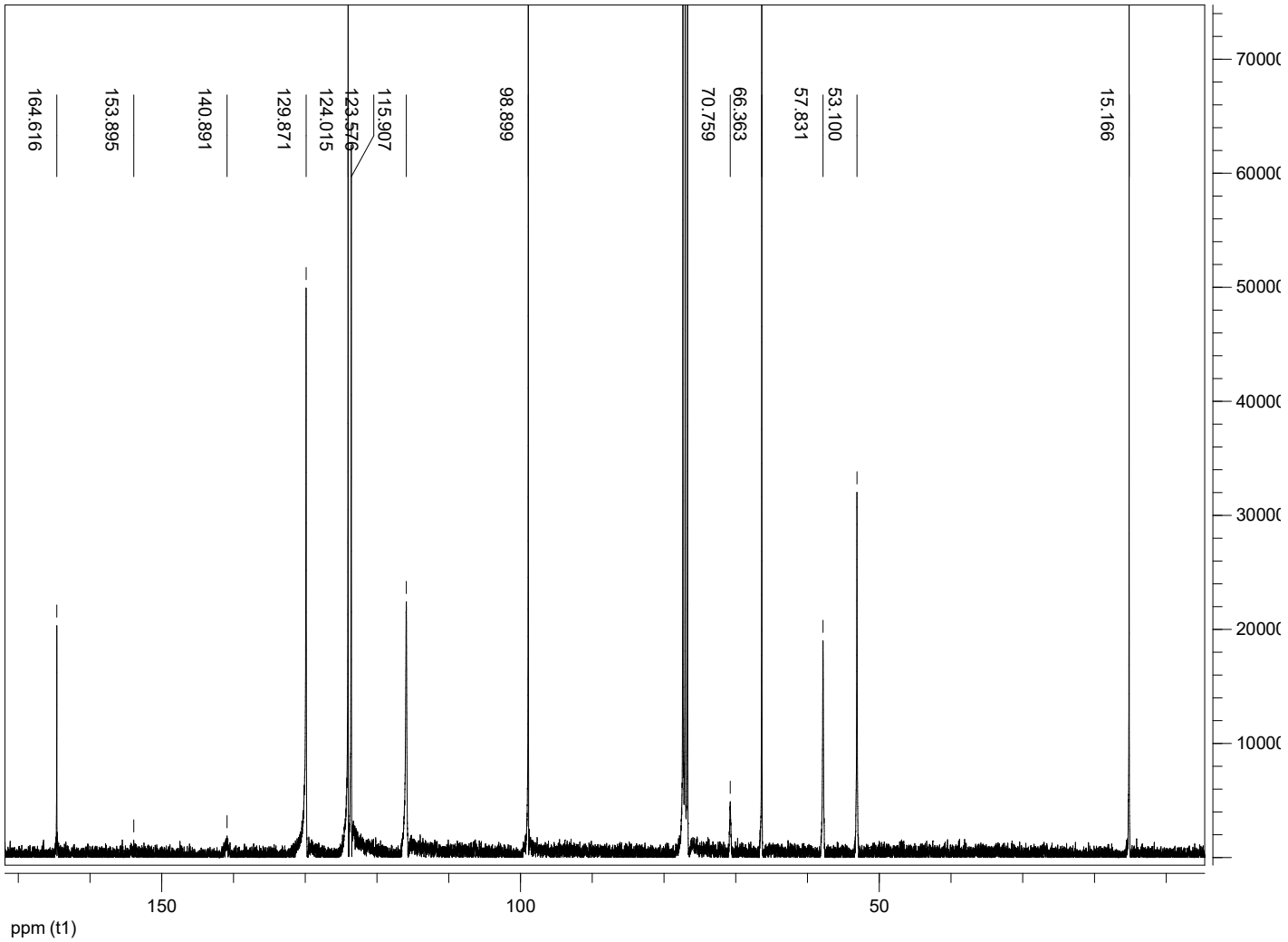


trans-(±)-**32a**

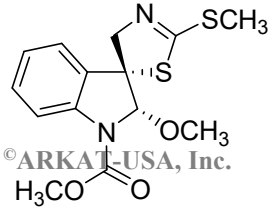
^{1}H NMR spectrum of ***trans*-(±)-32a** in $CDCl_3$



^{13}C NMR spectrum of ***trans*-(±)-32a** in $CDCl_3$

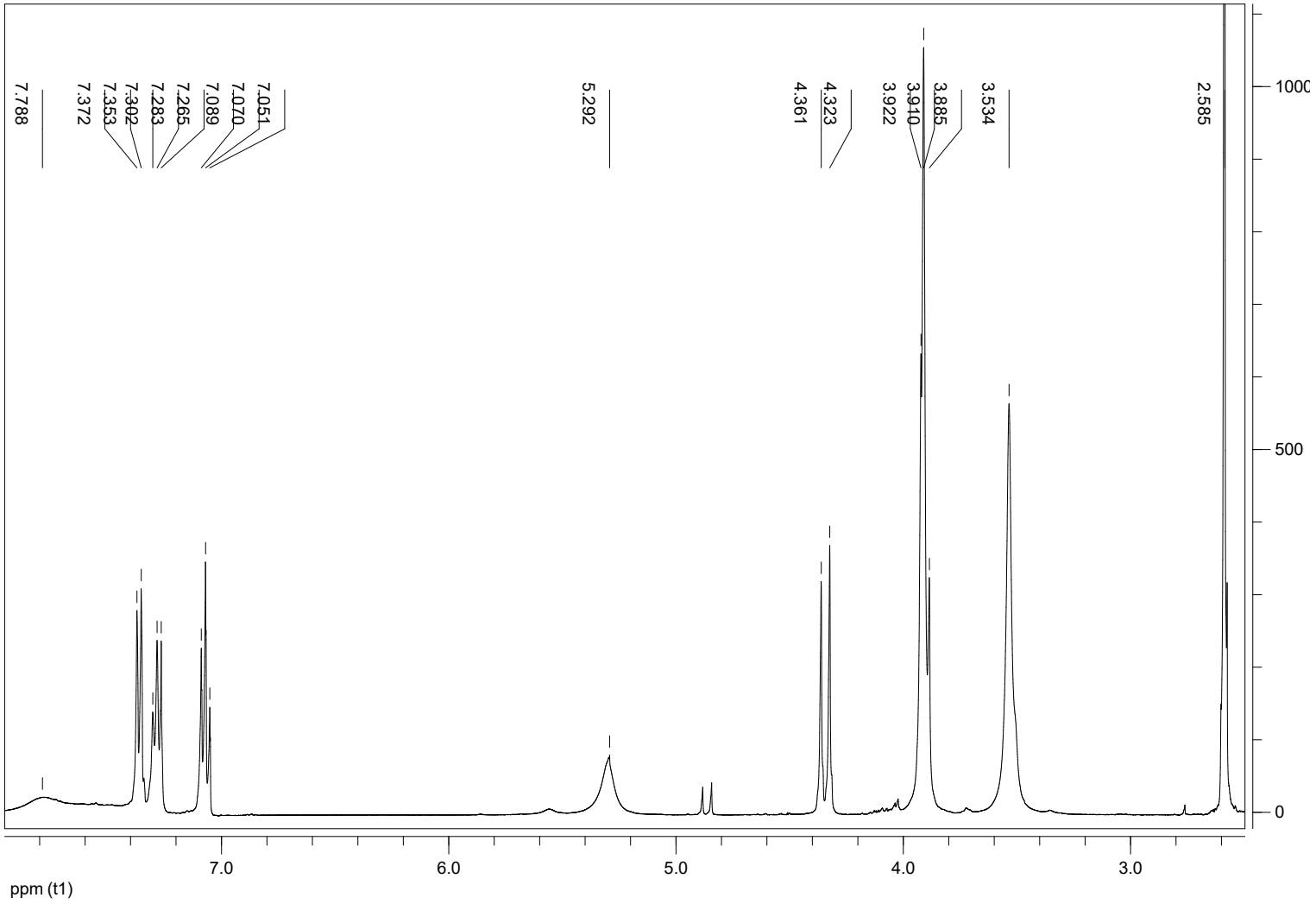


cis-(±)-1-Methoxycarbonylspirobrasinol methyl ether [(±)-32b]

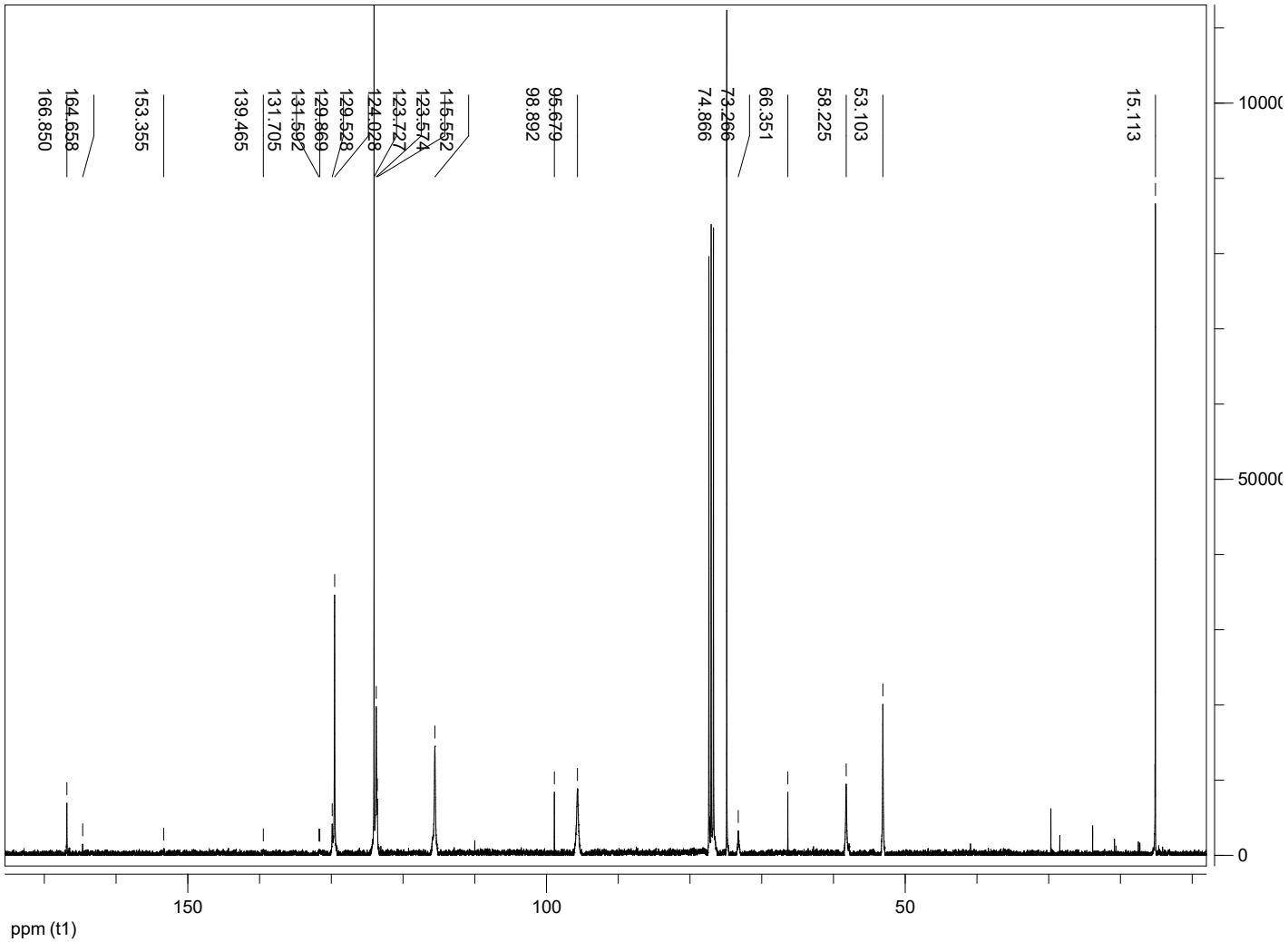


cis-(±)-**32b**

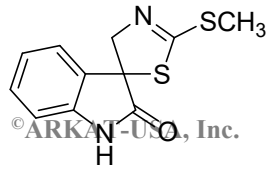
^{1}H NMR spectrum of ***cis*-(±)-32b** in $CDCl_3$



^{13}C NMR spectrum of ***cis*-(±)-32b** in $CDCl_3$

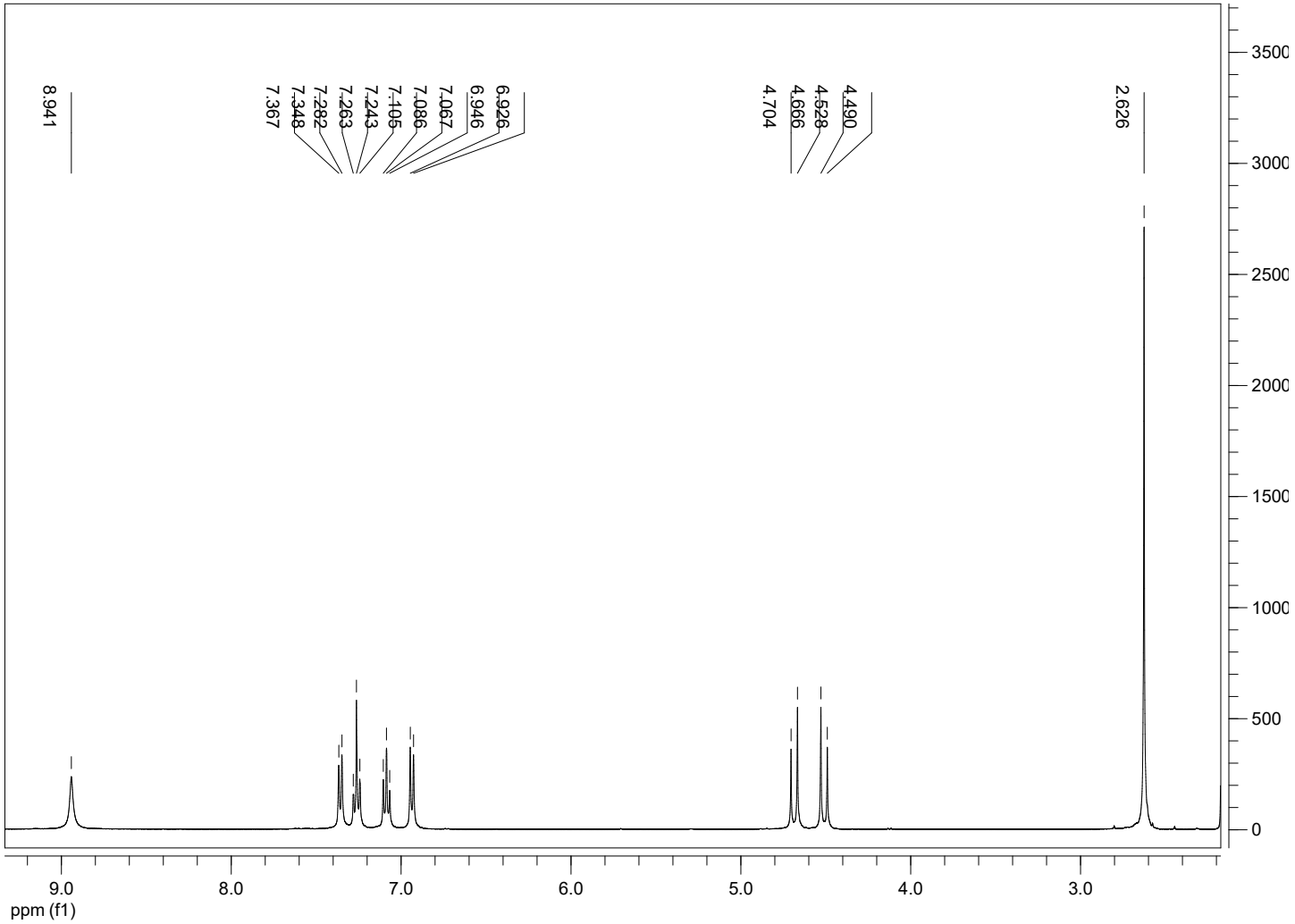


Spirobrassinin [(±)-1]

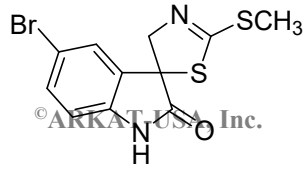


(±)-**1**

^{1}H NMR spectrum of (±)-**1**

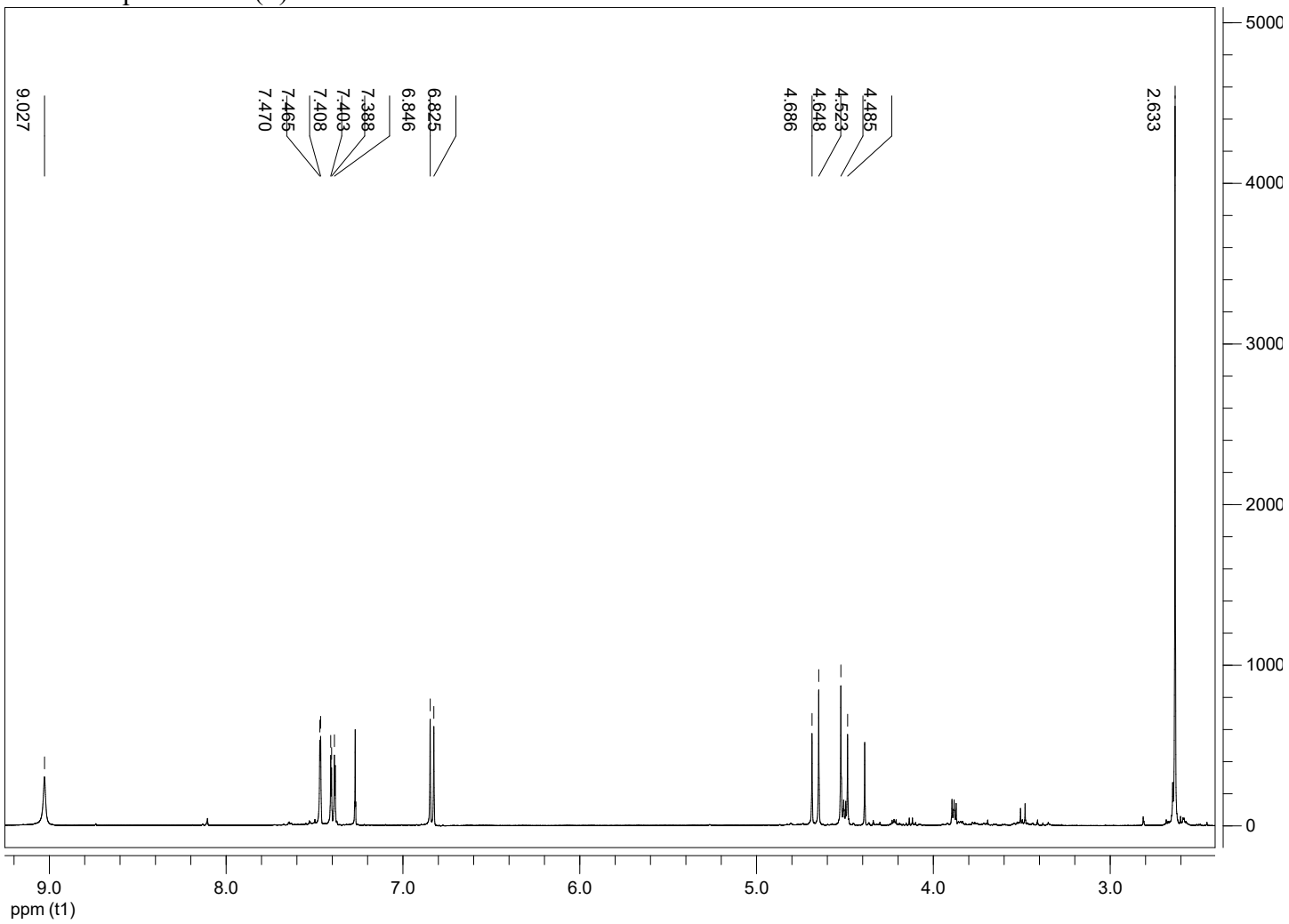


5-Bromospirobrassinin [(±)-43]

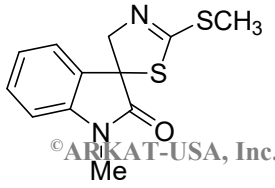


(±)-**43**

^{1}H NMR spectrum of (±)-**43**



1-Methylspirobrassinin [(±)-44]



(±)-**44**

^{1}H NMR spectrum of (±)-**44**