

## Electronic Supplementary Information

### Diastereoselective synthesis of 3-acetoxy-4-(3-aryloxiran-2-yl)azetidin-2-ones and their transformation into 3,4-oxolane-fused bicyclic $\beta$ -lactams

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#### Contents

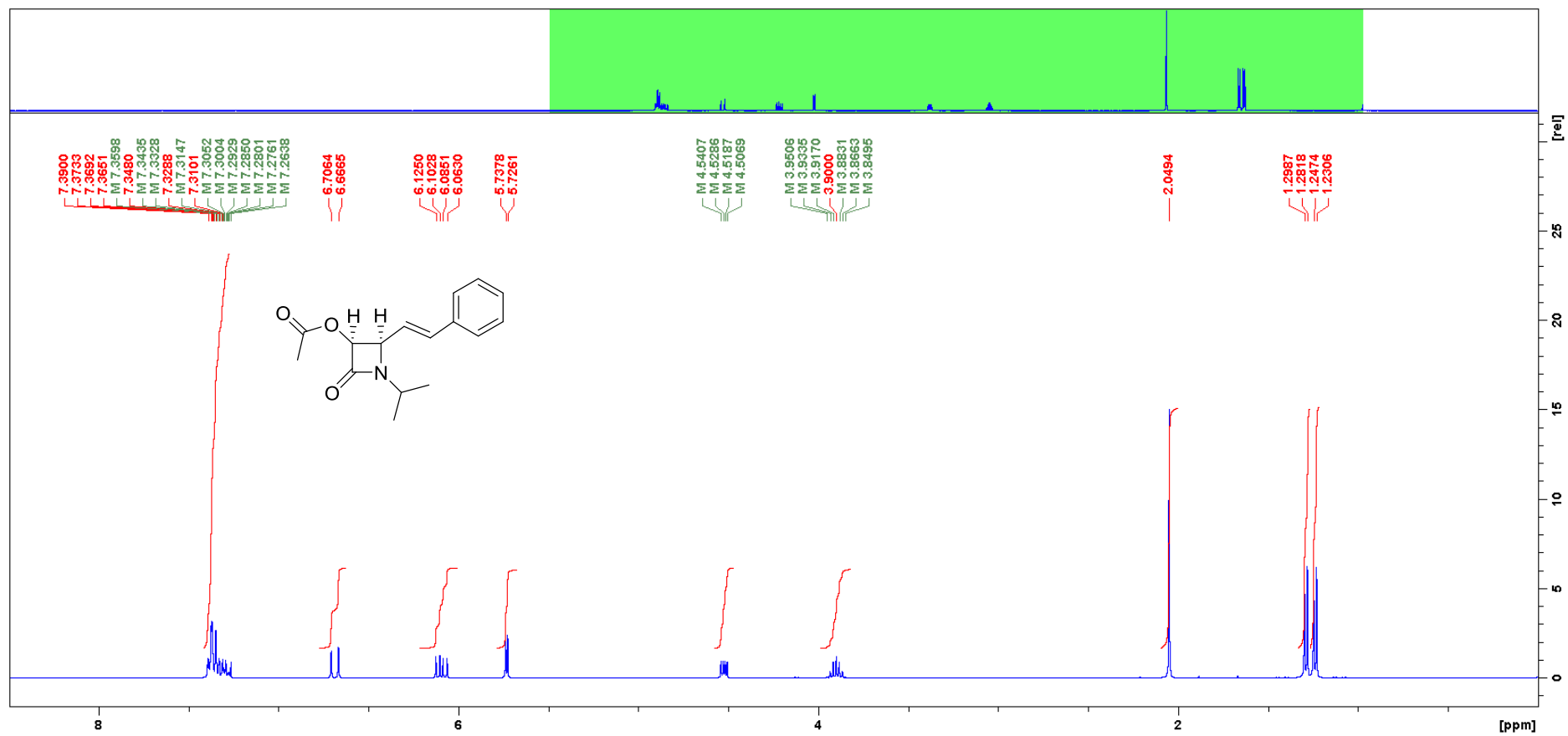
<sup>1</sup>H and <sup>13</sup>C NMR spectra of all new compounds:

Compound <b>3</b>	2
Compound <b>5a</b>	4
Compounds <b>9a,c-e</b>	6
Compounds <b>4a-e</b>	14
Compounds <b>11a-e</b>	24
Compound <b>12a</b>	34
Compounds <b>13a-b</b>	36

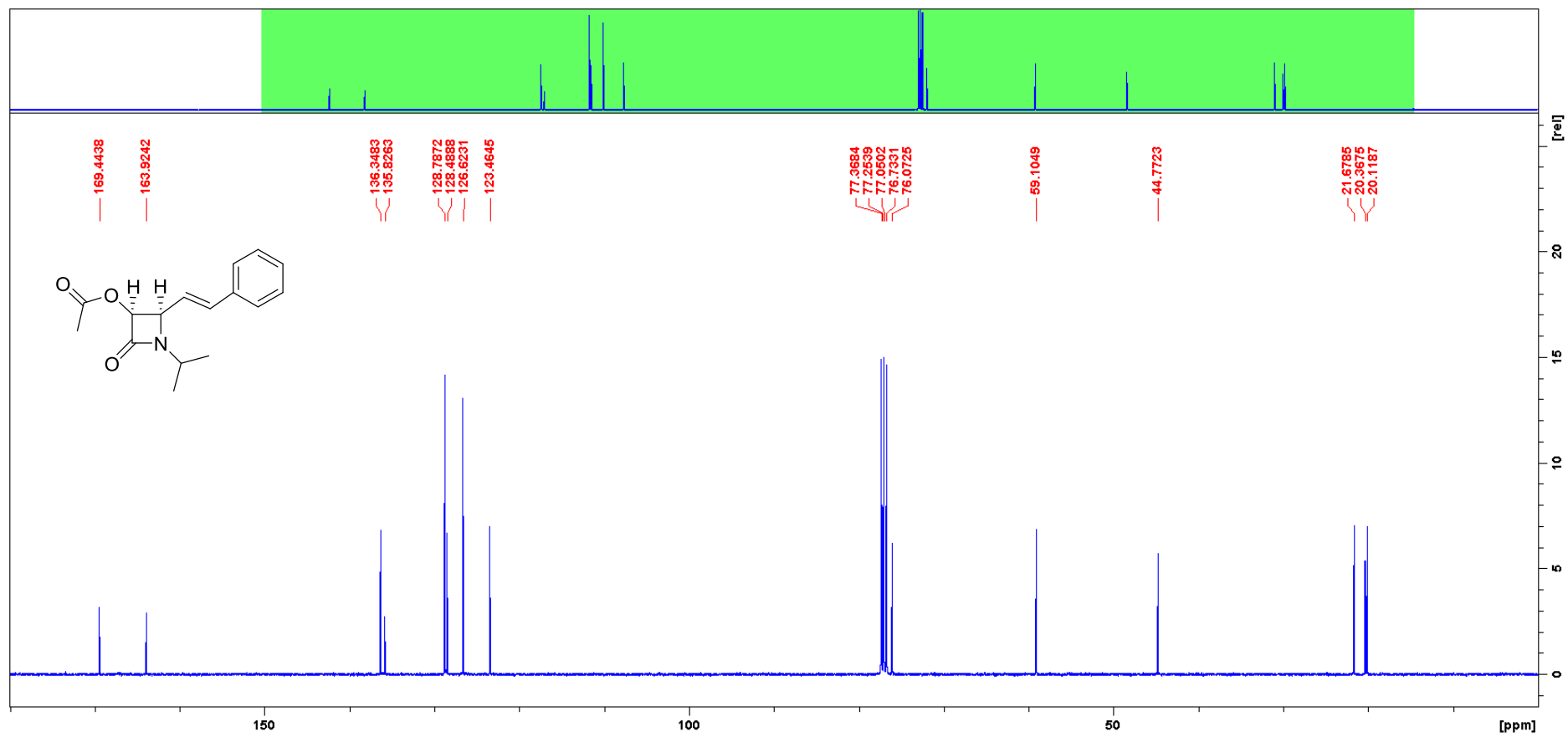
Single crystal X-ray diffraction:

Compounds <b>11b, 12a</b>	40
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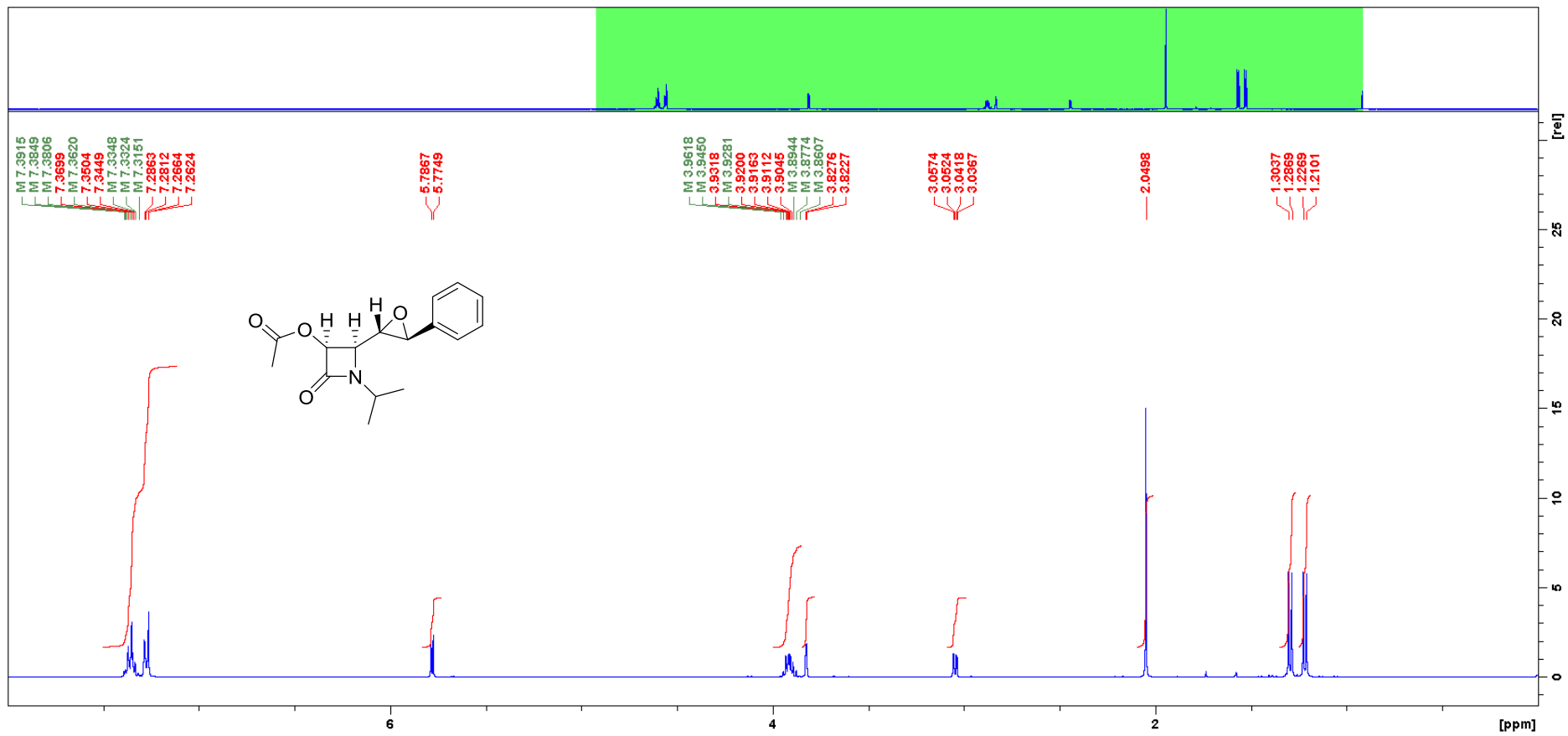
Compound 3: <sup>1</sup>H NMR



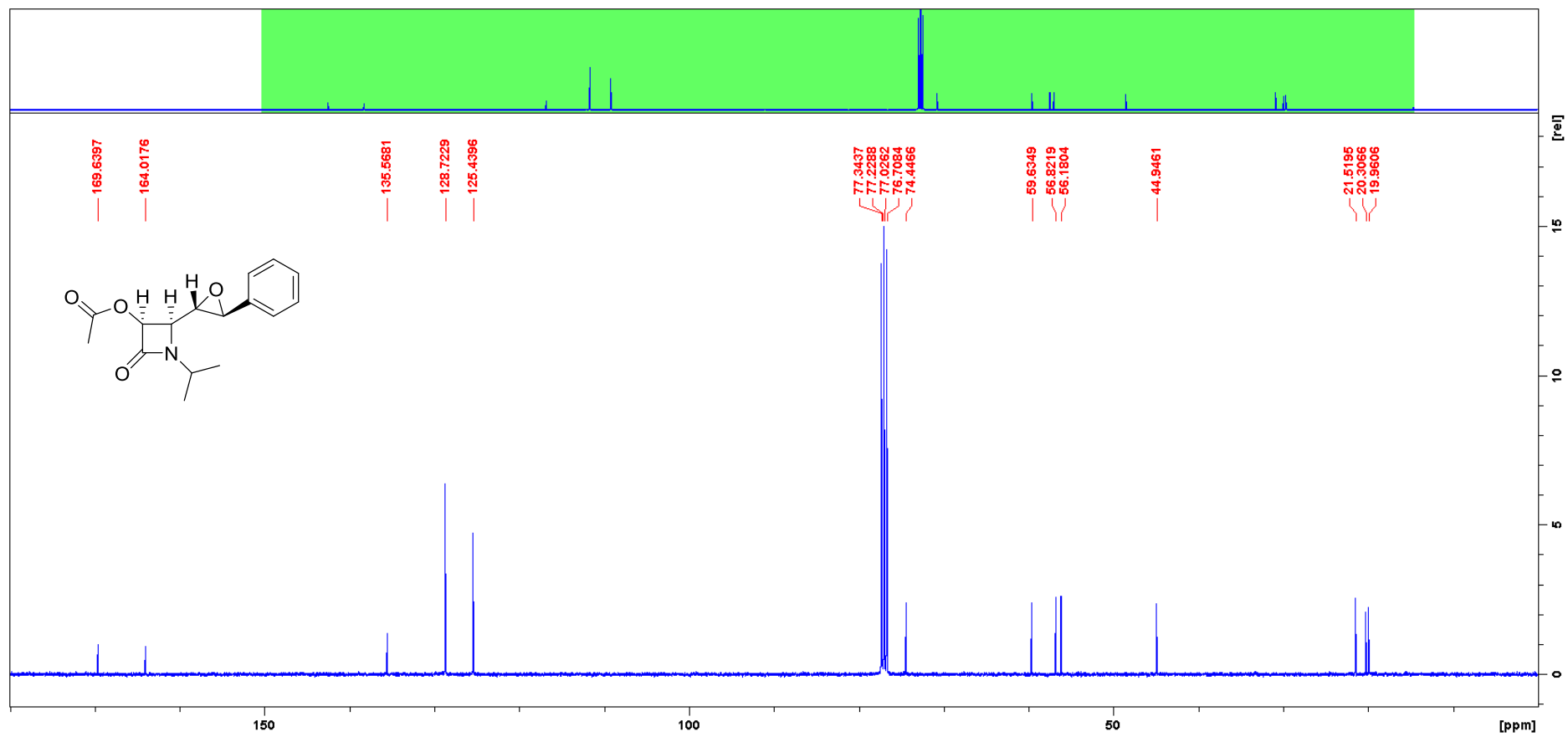
Compound 3:  $^{13}\text{C}$  NMR



Compound 5a: <sup>1</sup>H NMR

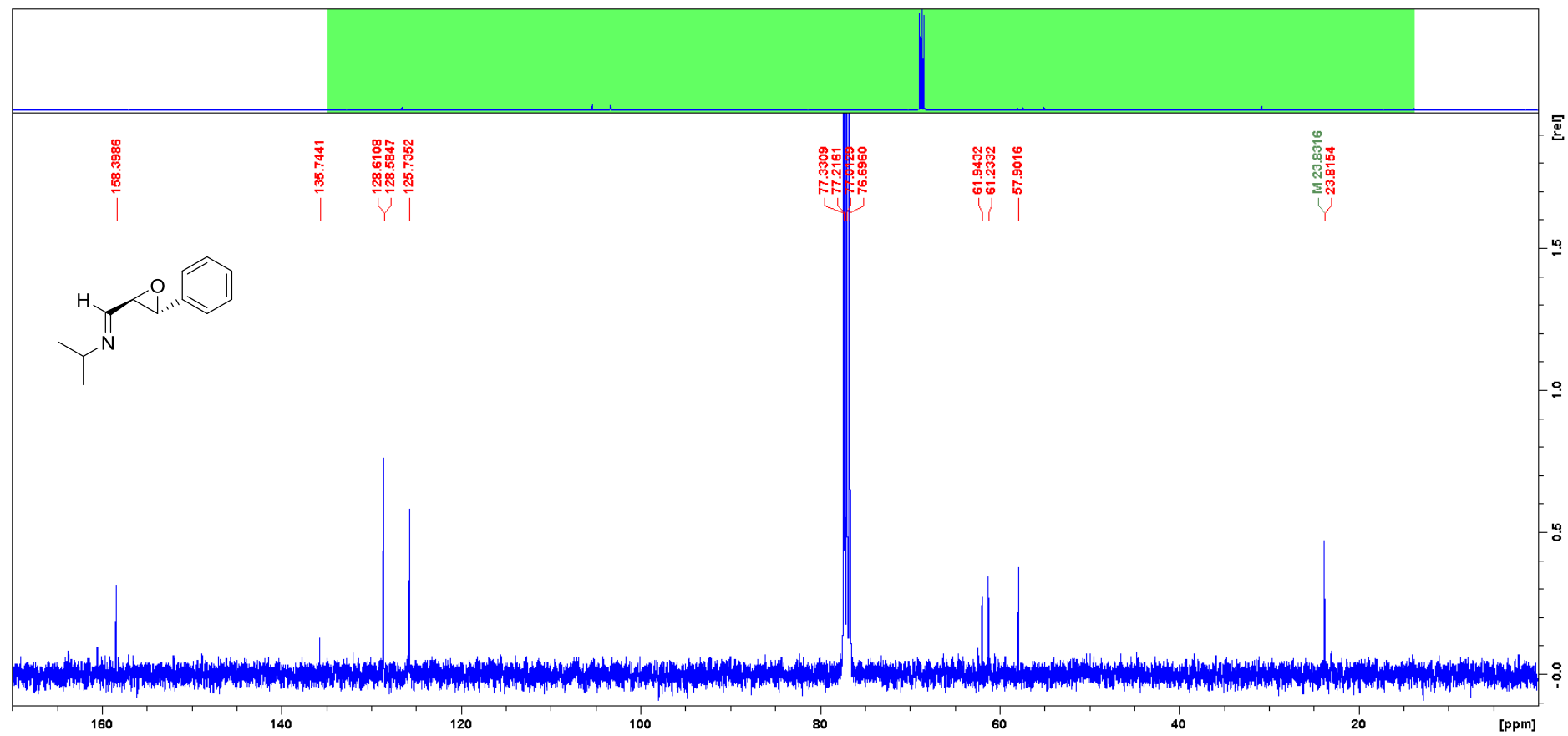


Compound 5a:  $^{13}\text{C}$  NMR

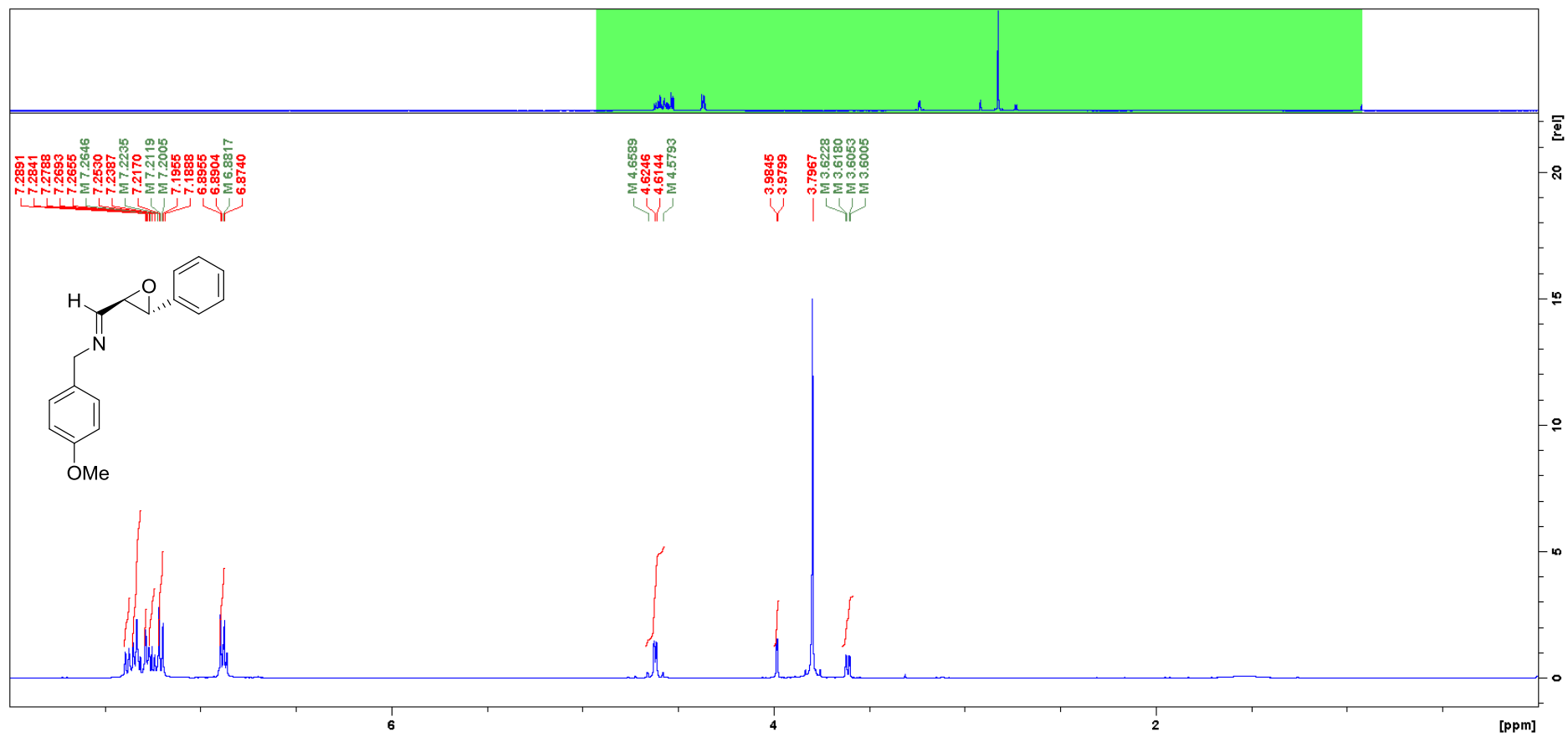




Compound **9a**:  $^{13}\text{C}$  NMR

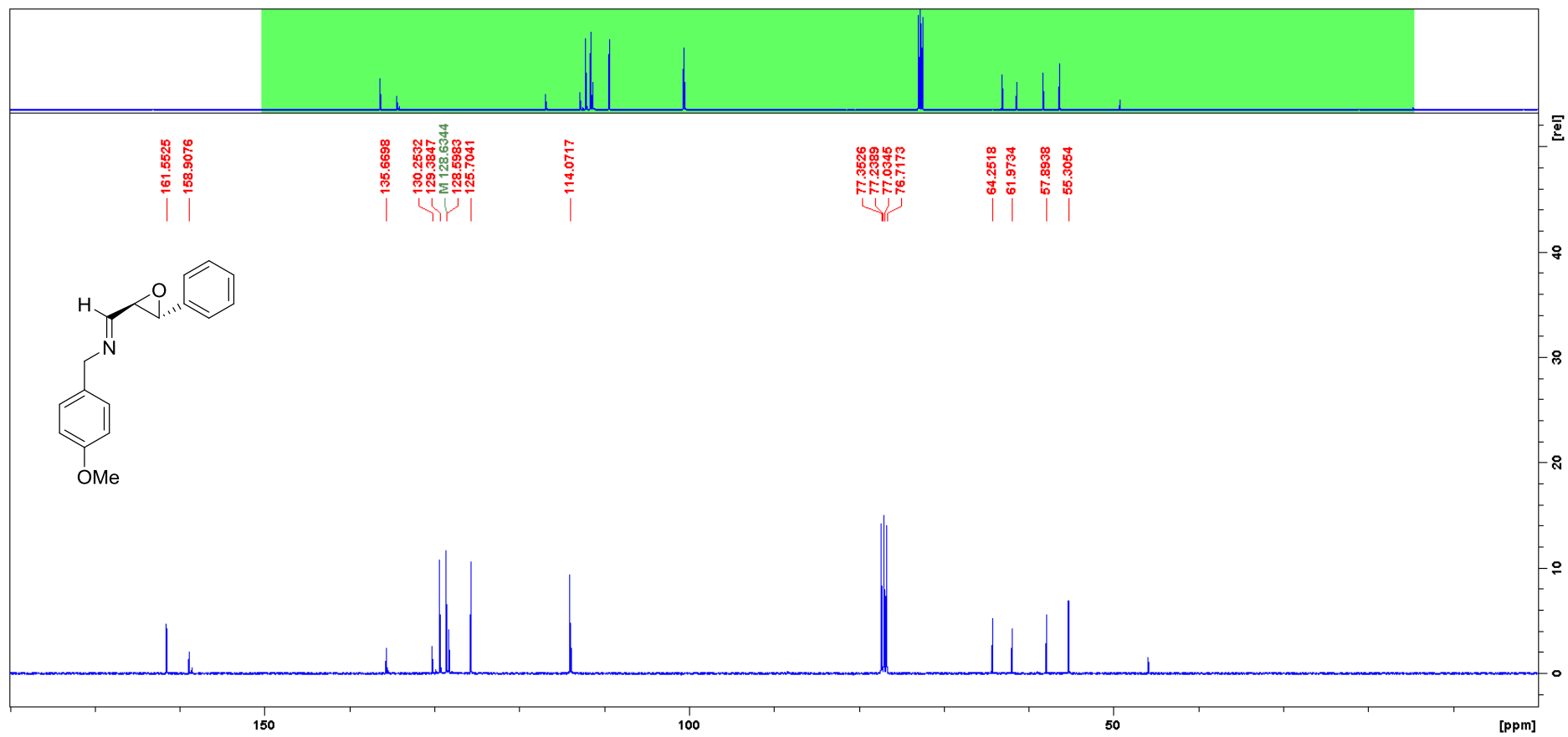


Compound 9c: <sup>1</sup>H NMR

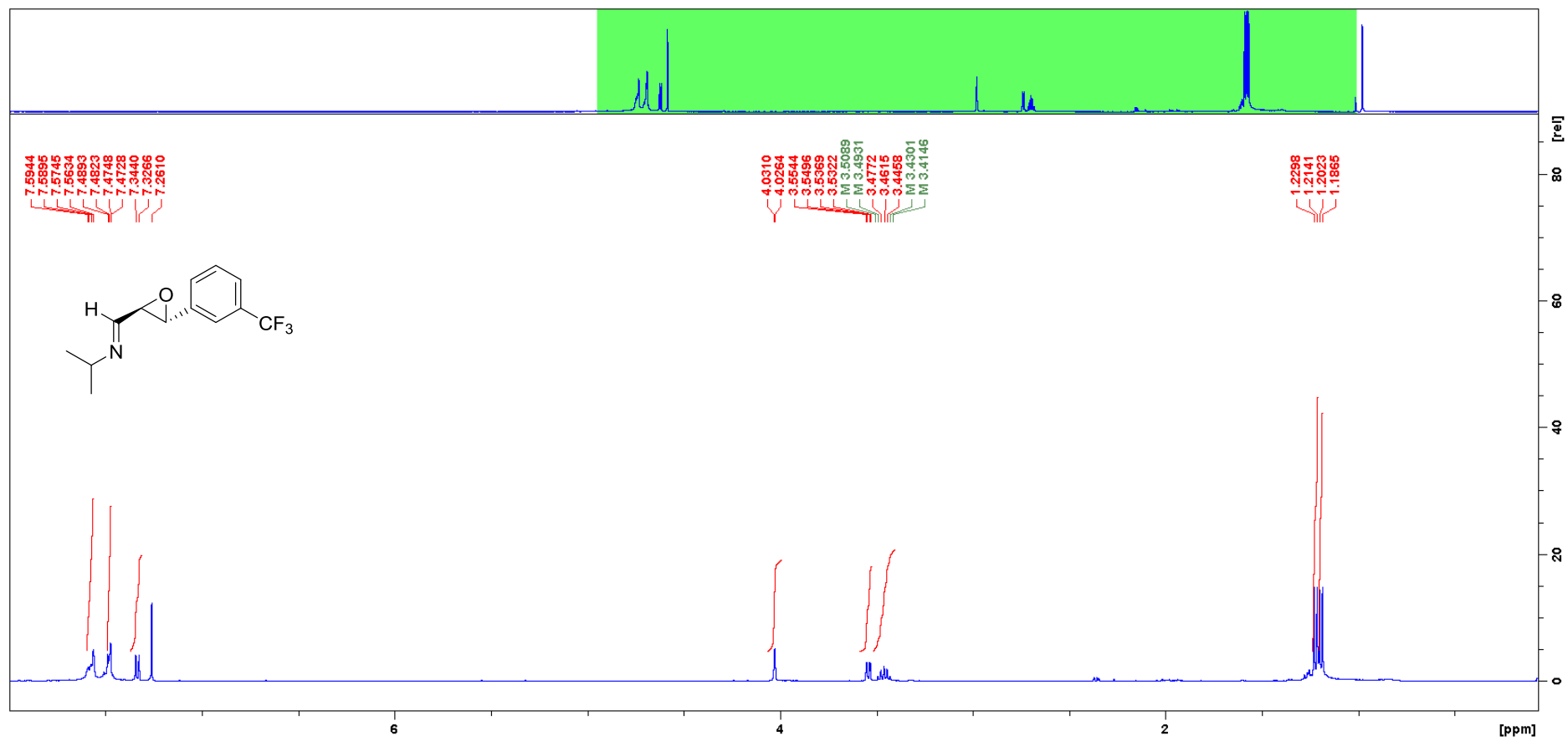




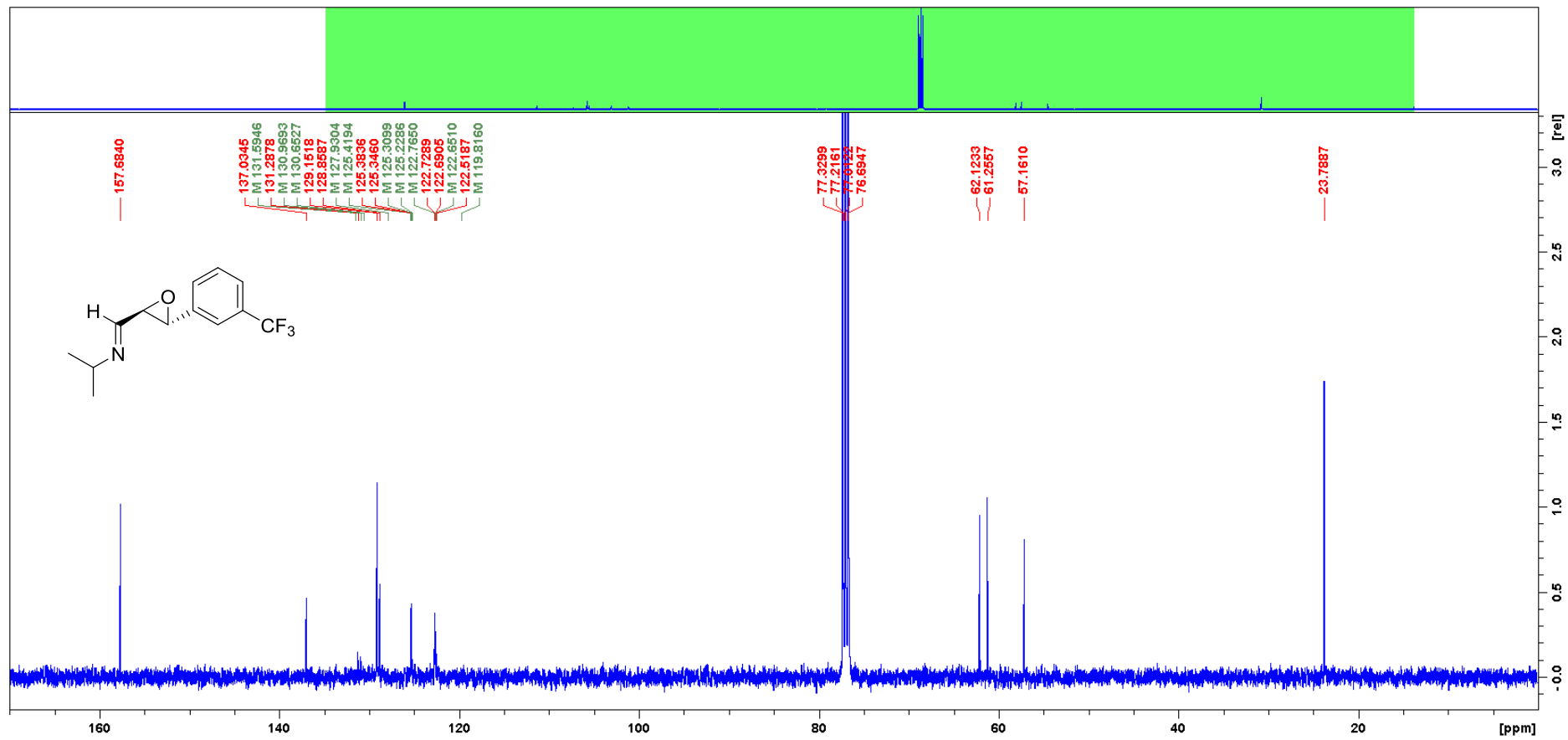
Compound **9c**:  $^{13}\text{C}$  NMR



Compound **9d**:  $^1\text{H}$  NMR

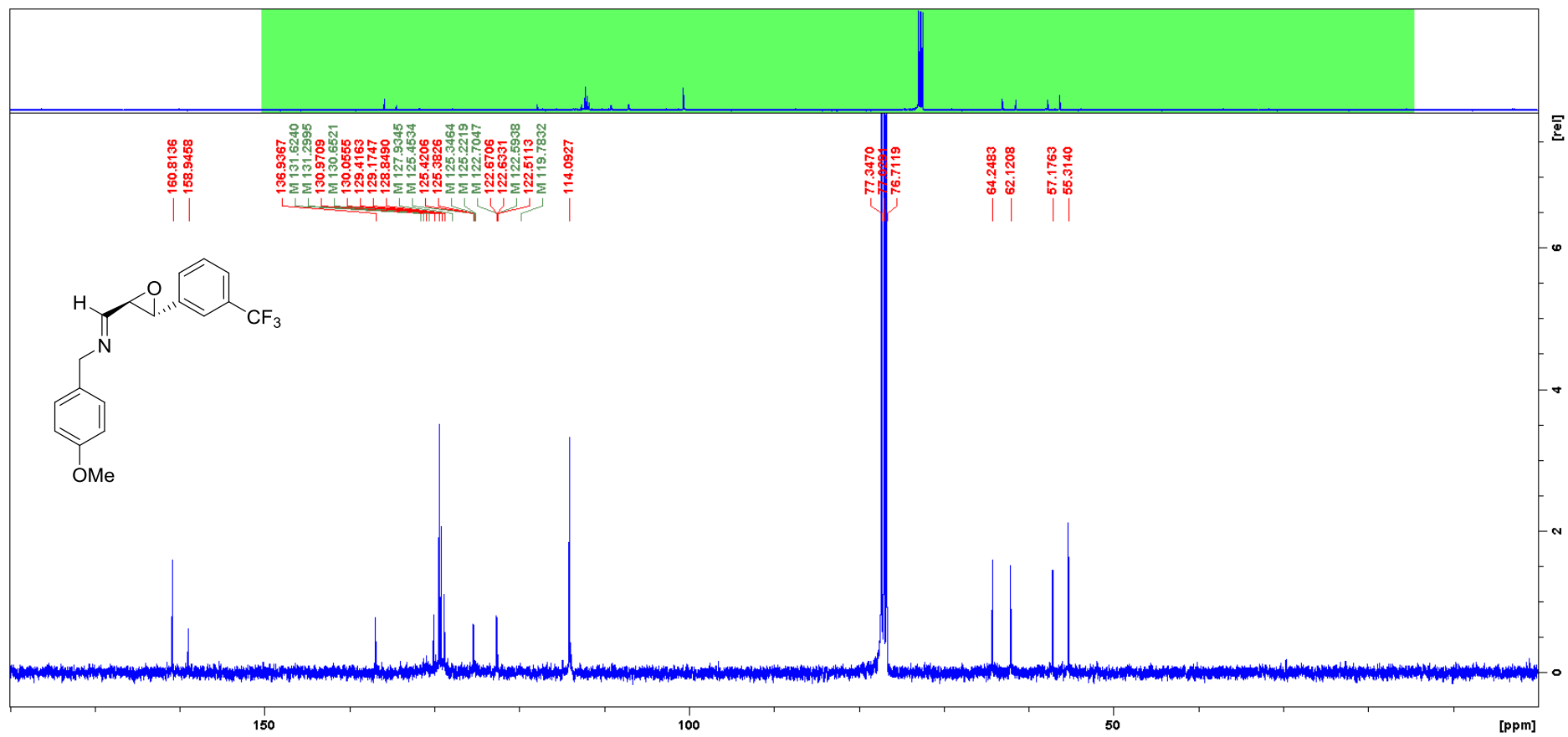


Compound **9d**:  $^{13}\text{C}$  NMR

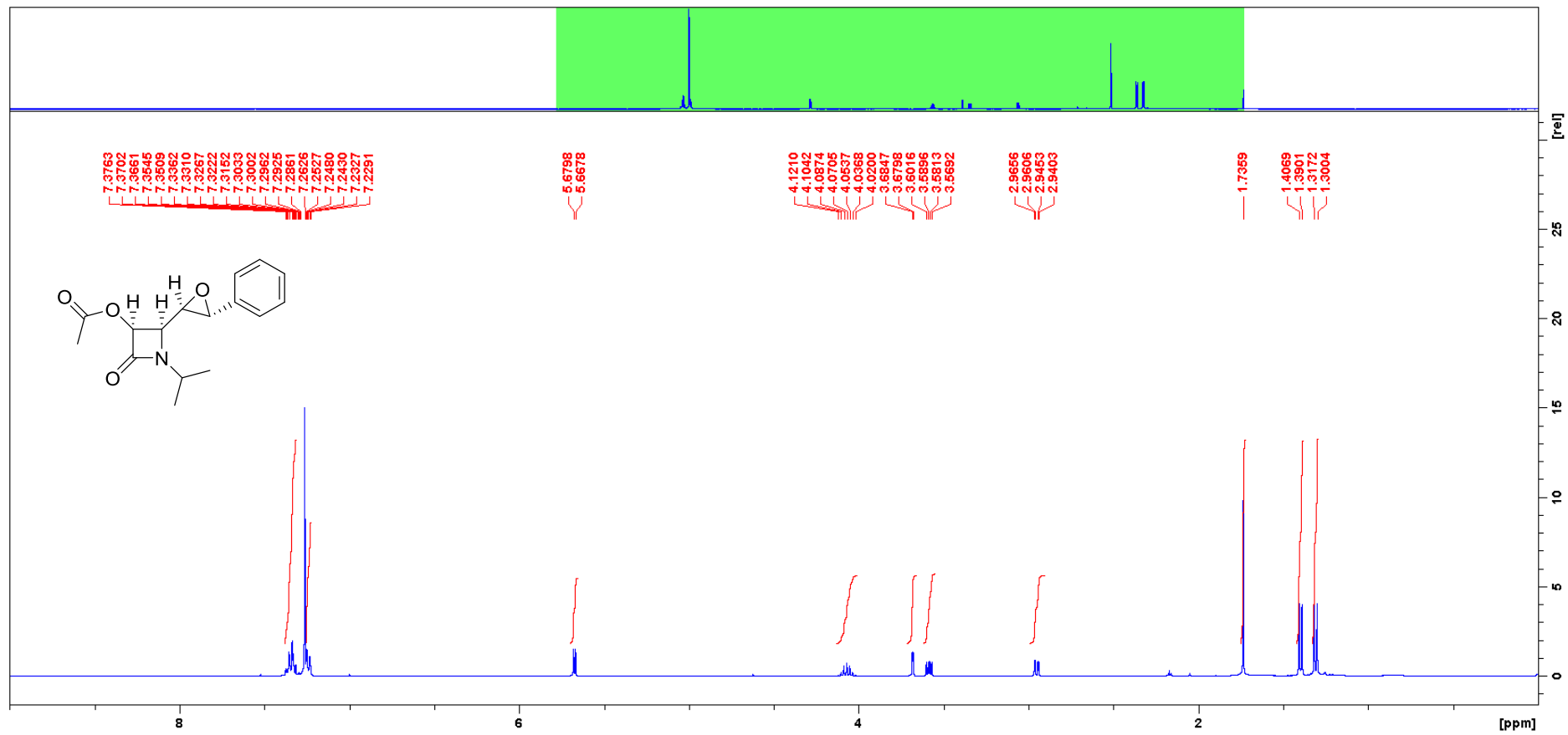




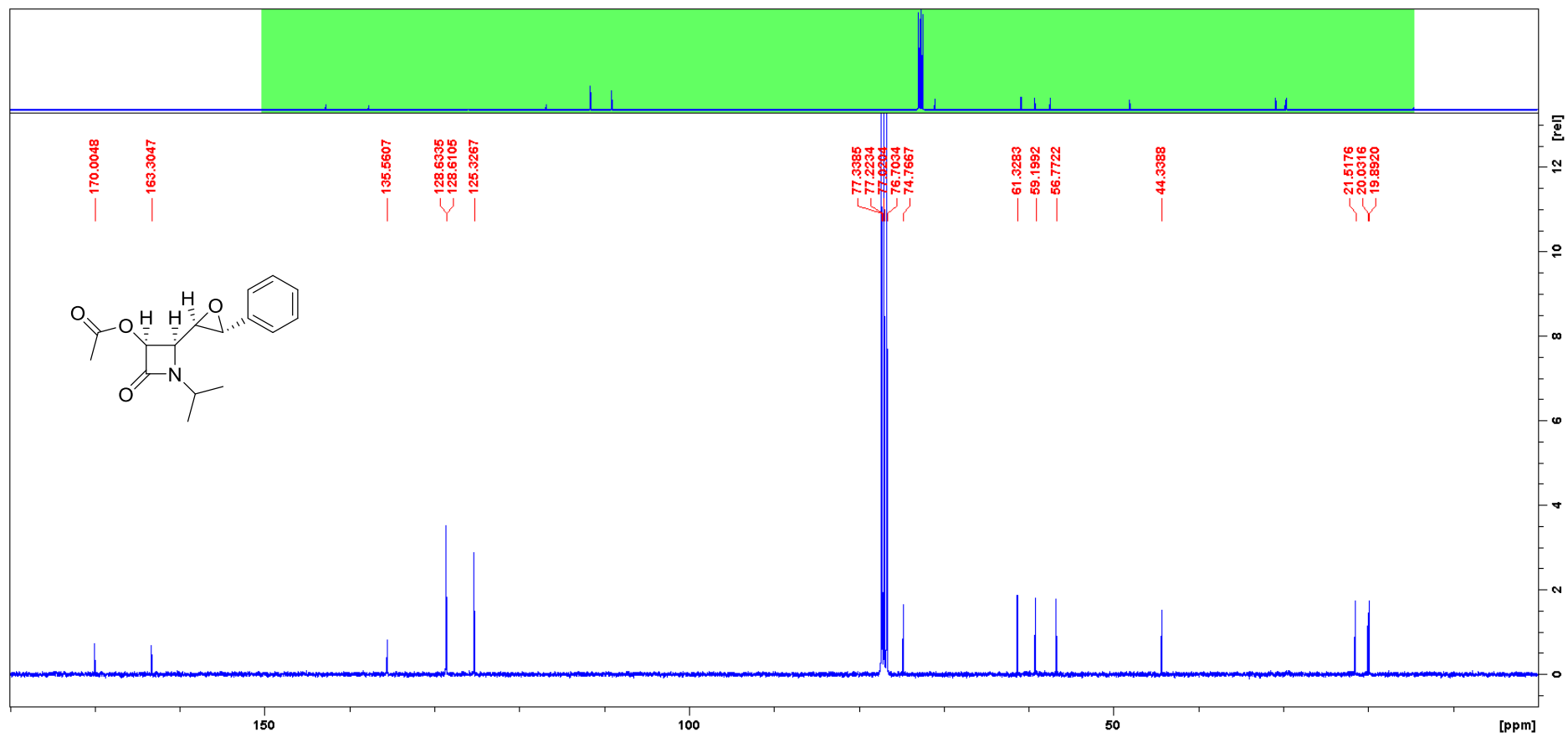
Compound 9e:  $^{13}\text{C}$  NMR



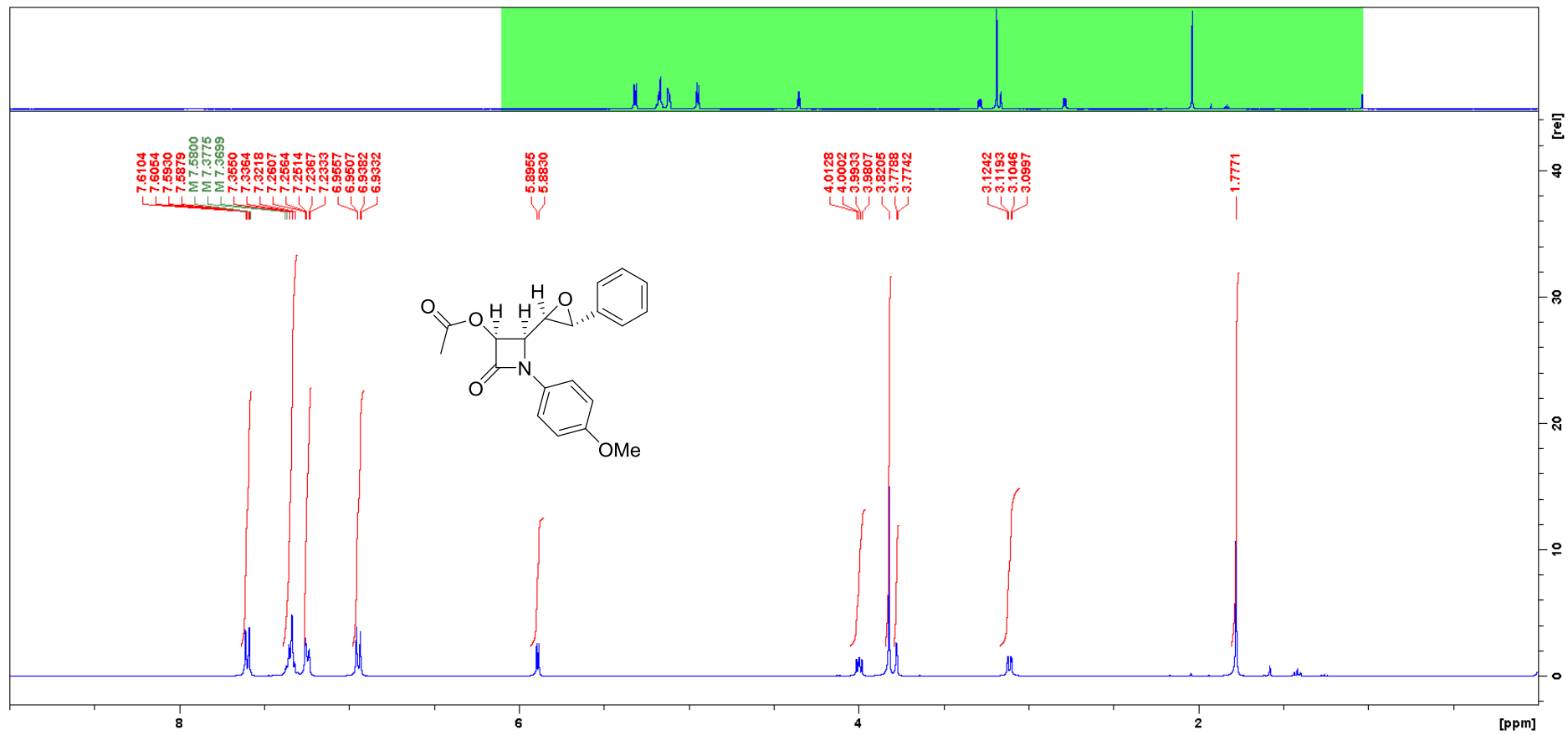
Compound 4a: <sup>1</sup>H NMR



Compound **4a**:  $^{13}\text{C}$  NMR

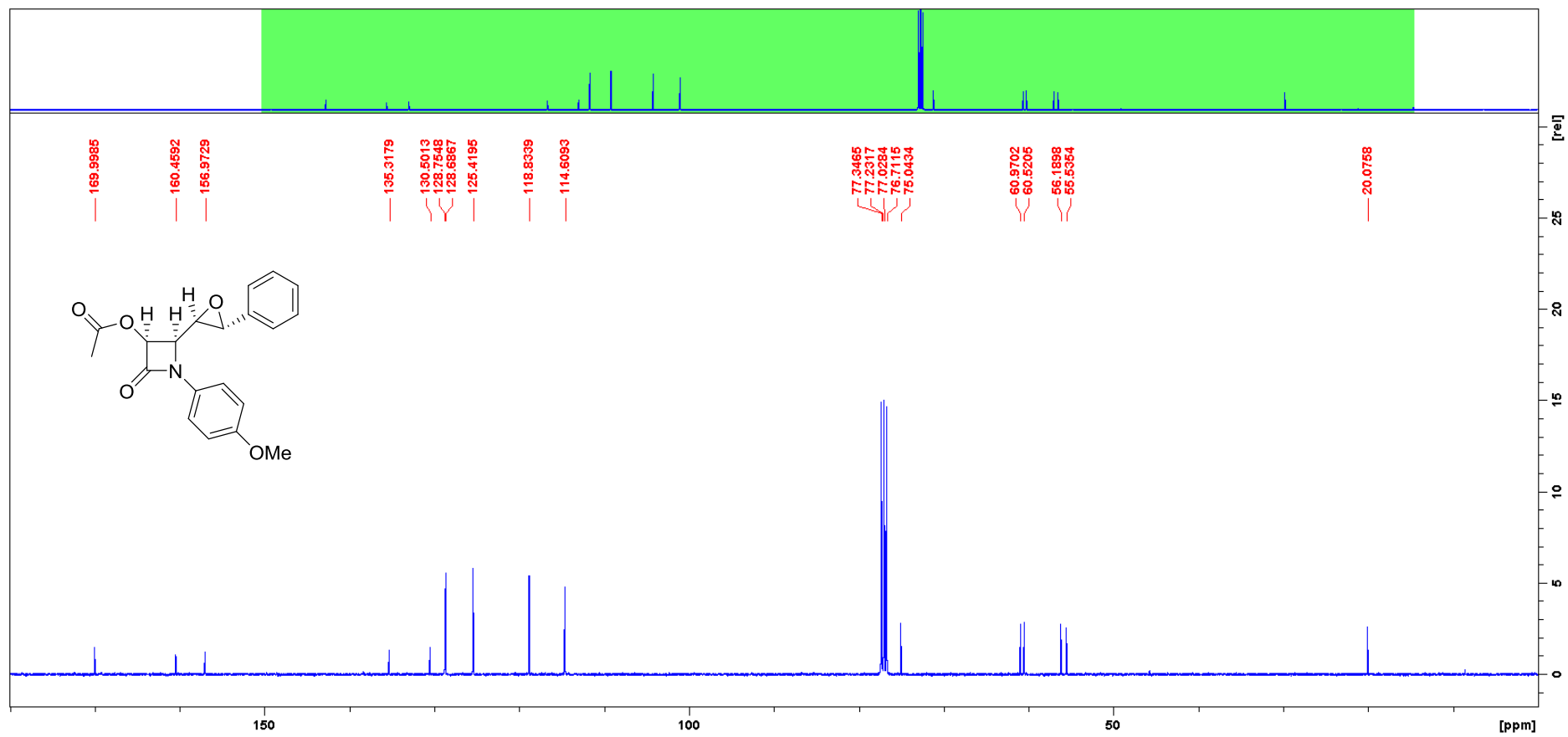


Compound **4b**:  $^1\text{H}$  NMR

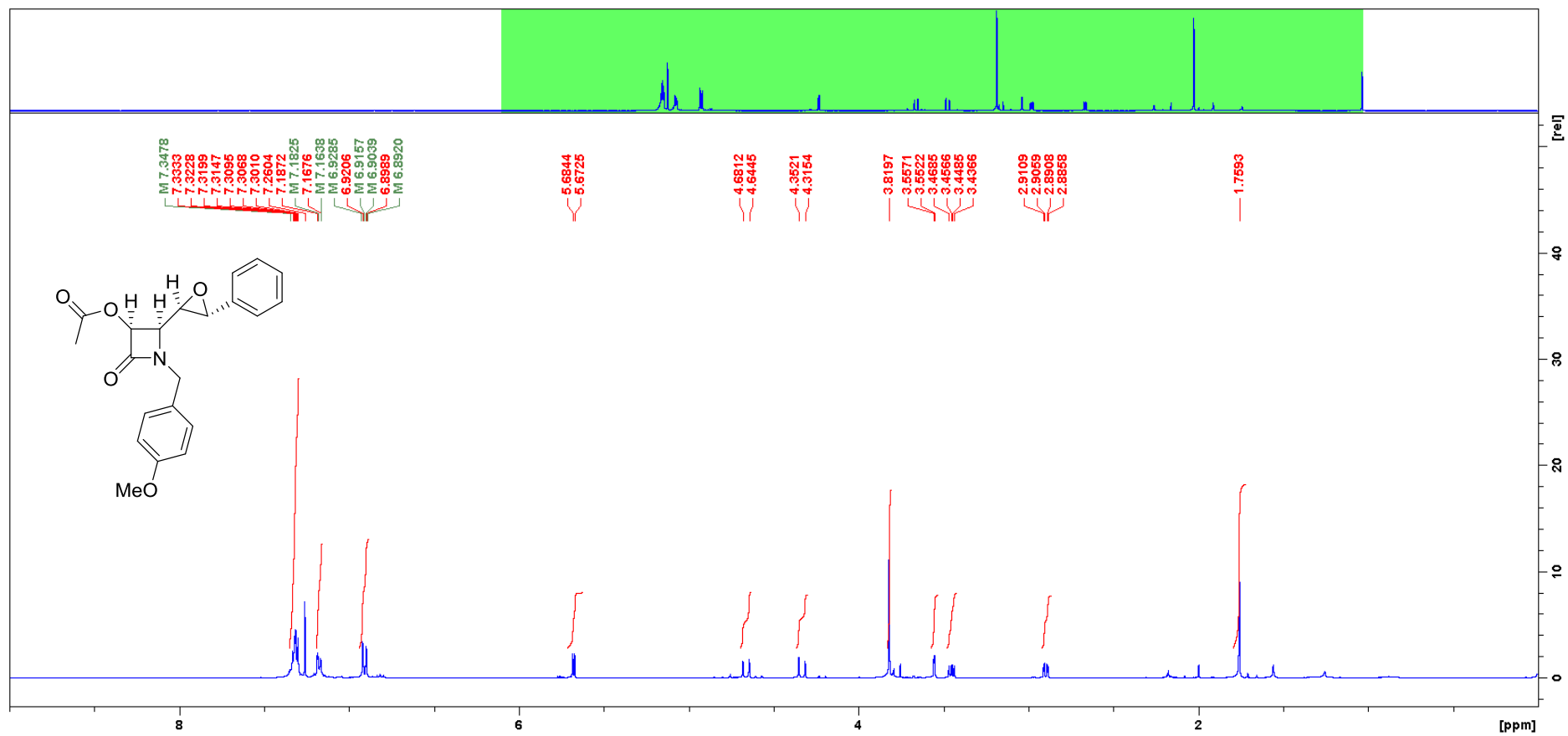




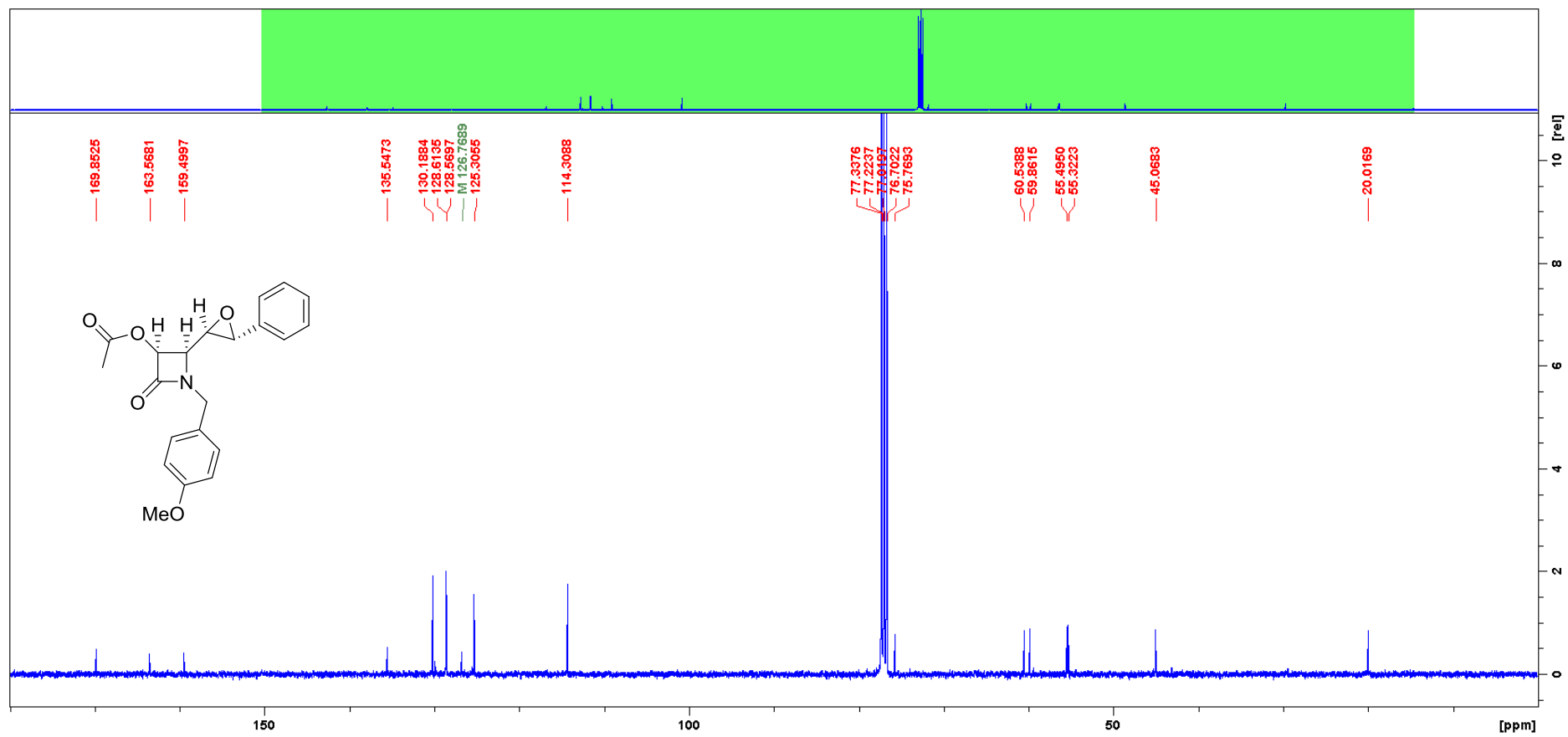
Compound **4b**:  $^{13}\text{C}$  NMR



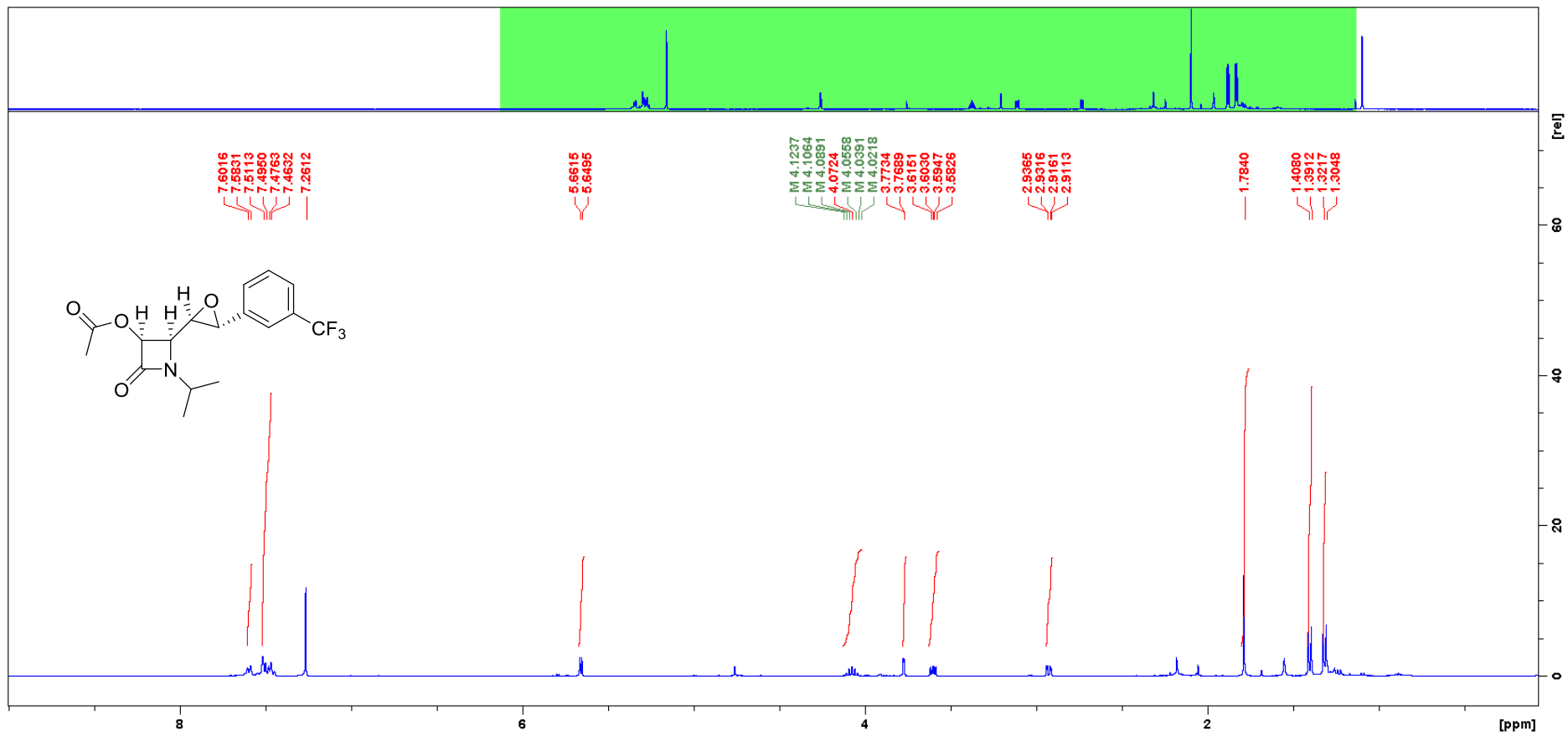
Compound 4c: <sup>1</sup>H NMR



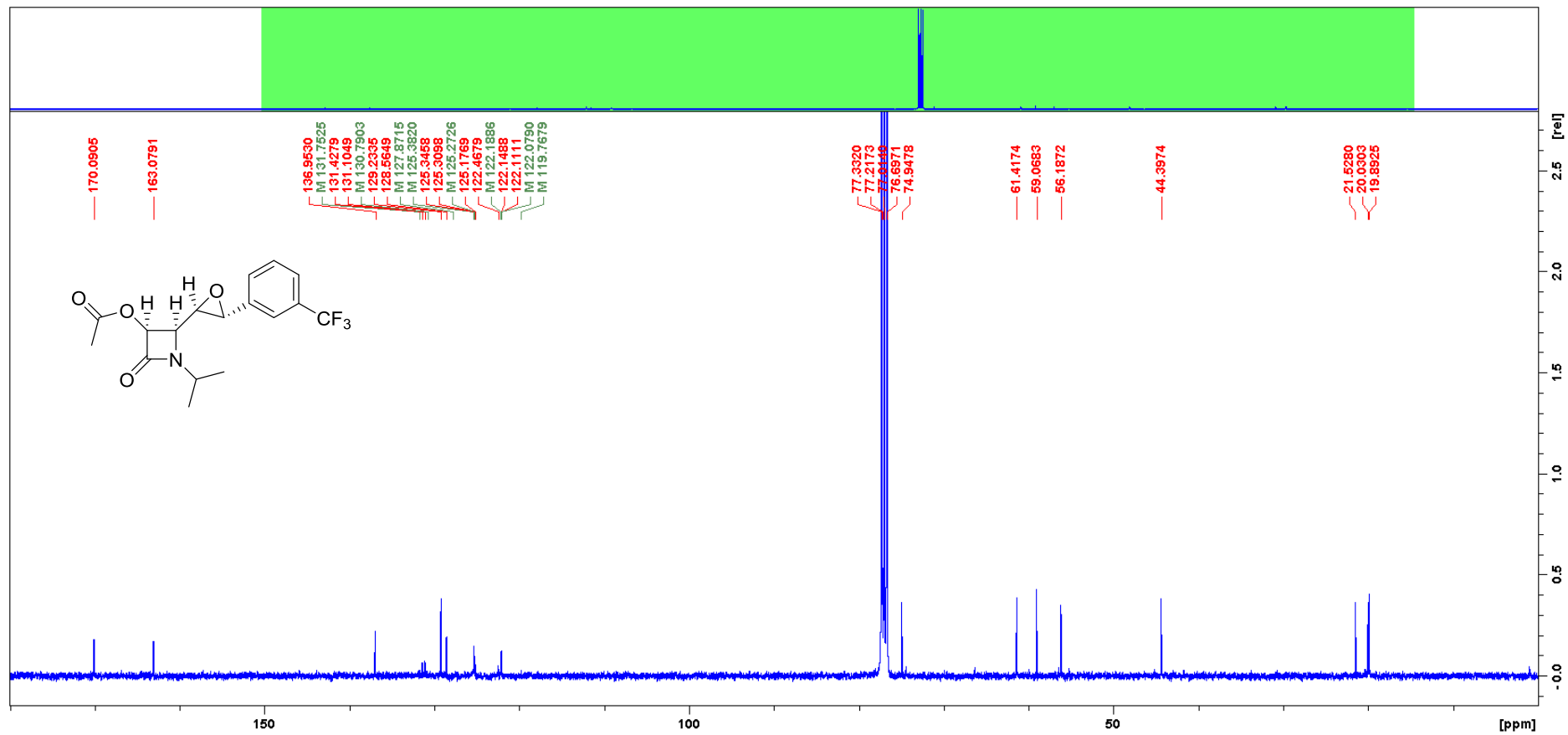
Compound 4c:  $^{13}\text{C}$  NMR



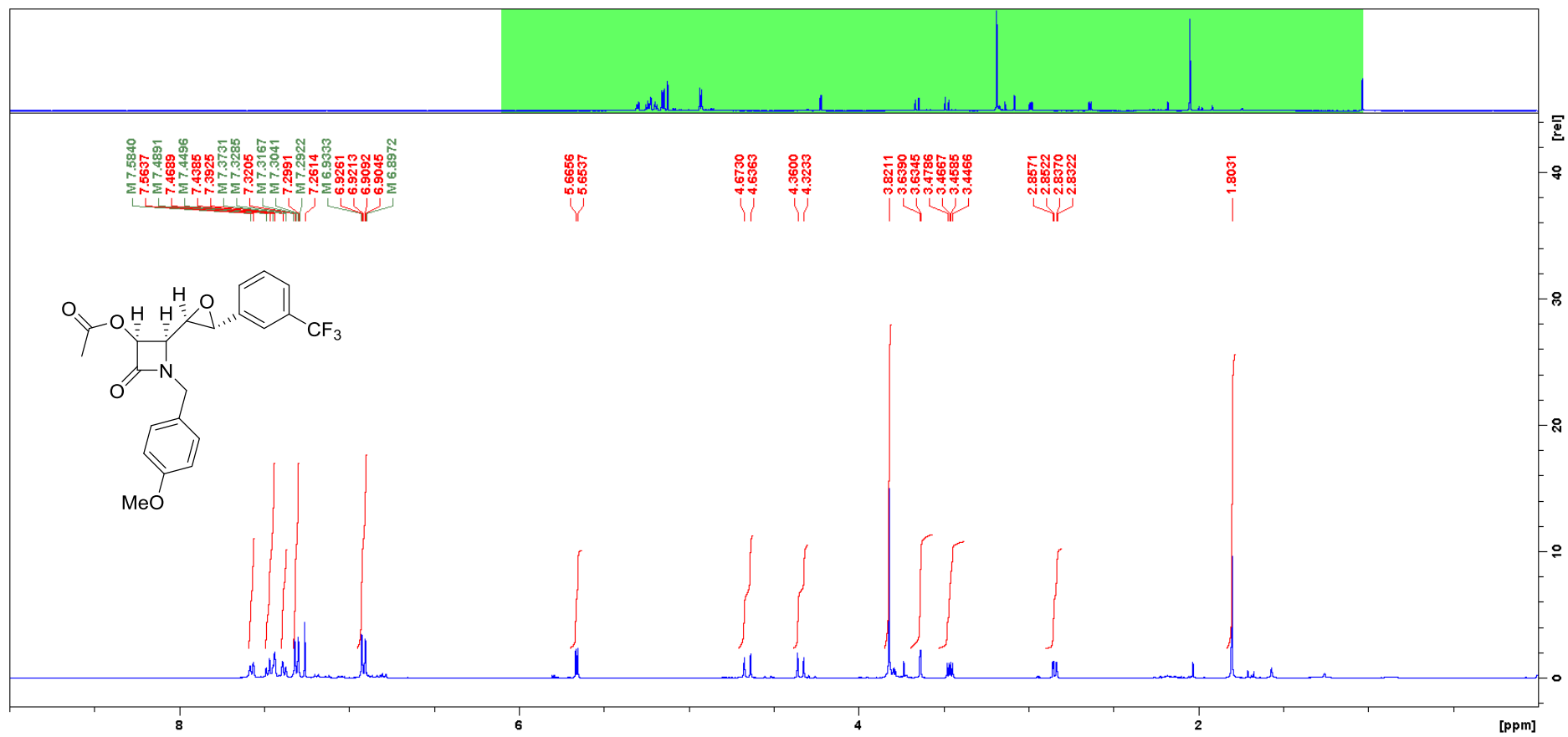
Compound **4d**: <sup>1</sup>H NMR



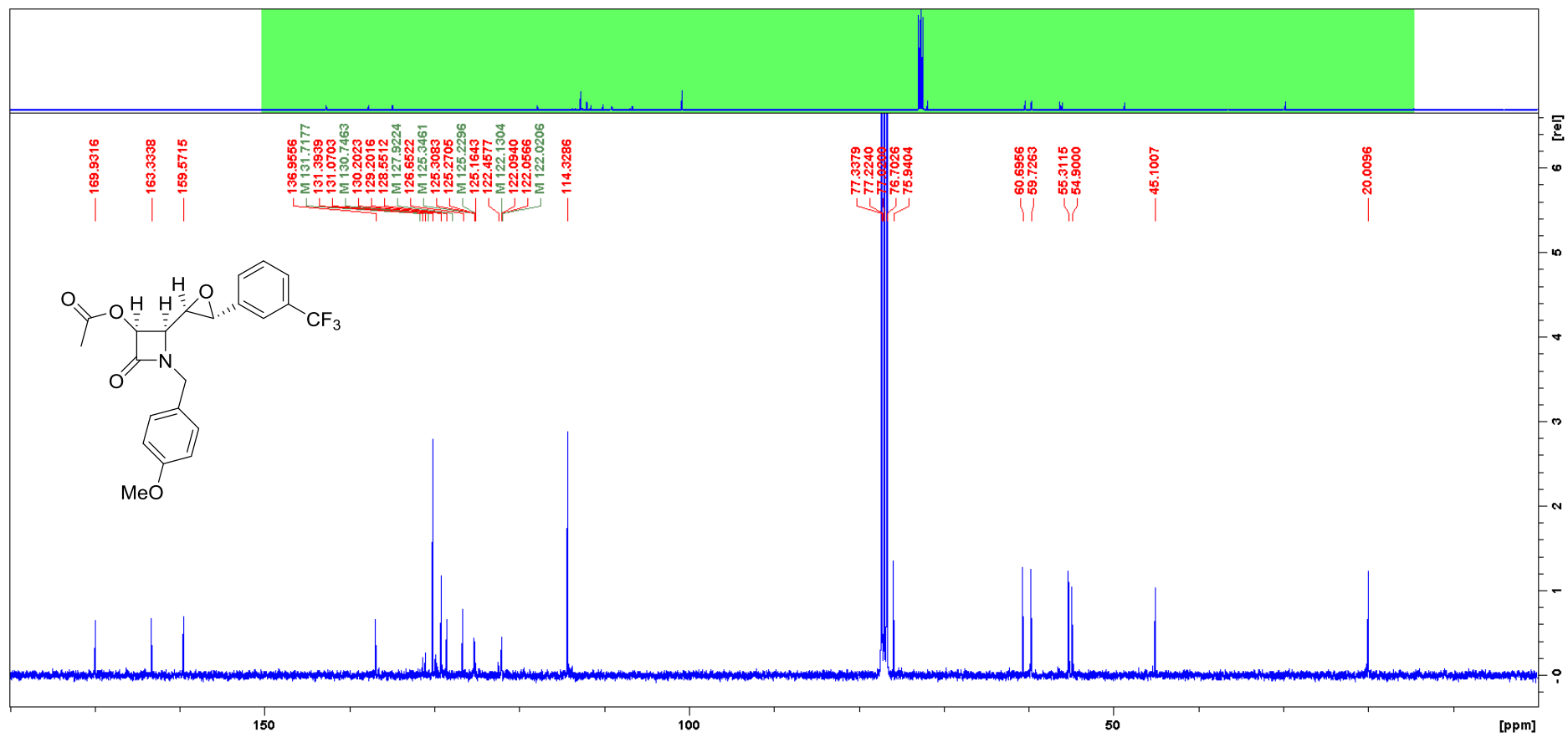
Compound **4d**:  $^{13}\text{C}$  NMR



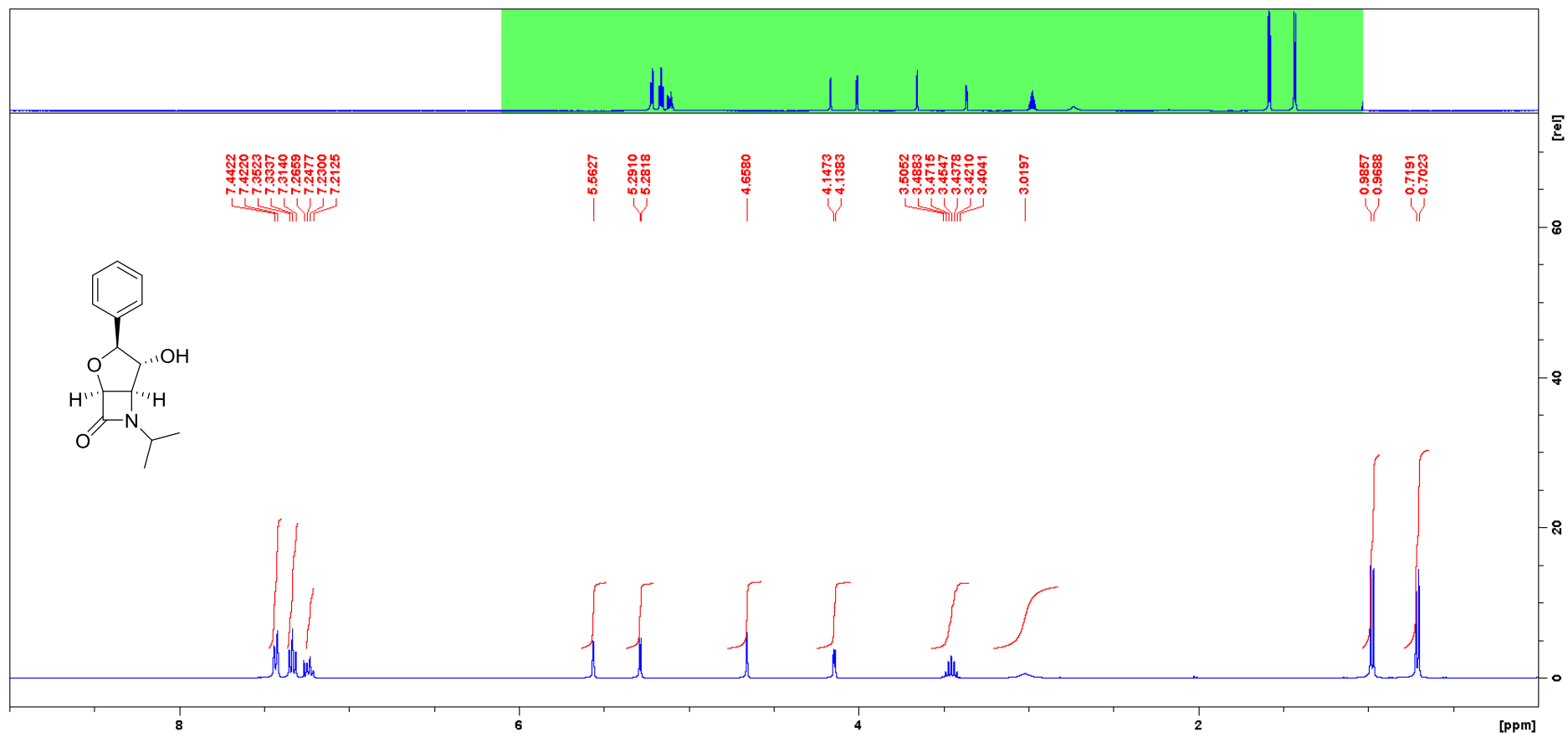
Compound 4e: <sup>1</sup>H NMR



Compound 4e:  $^{13}\text{C}$  NMR

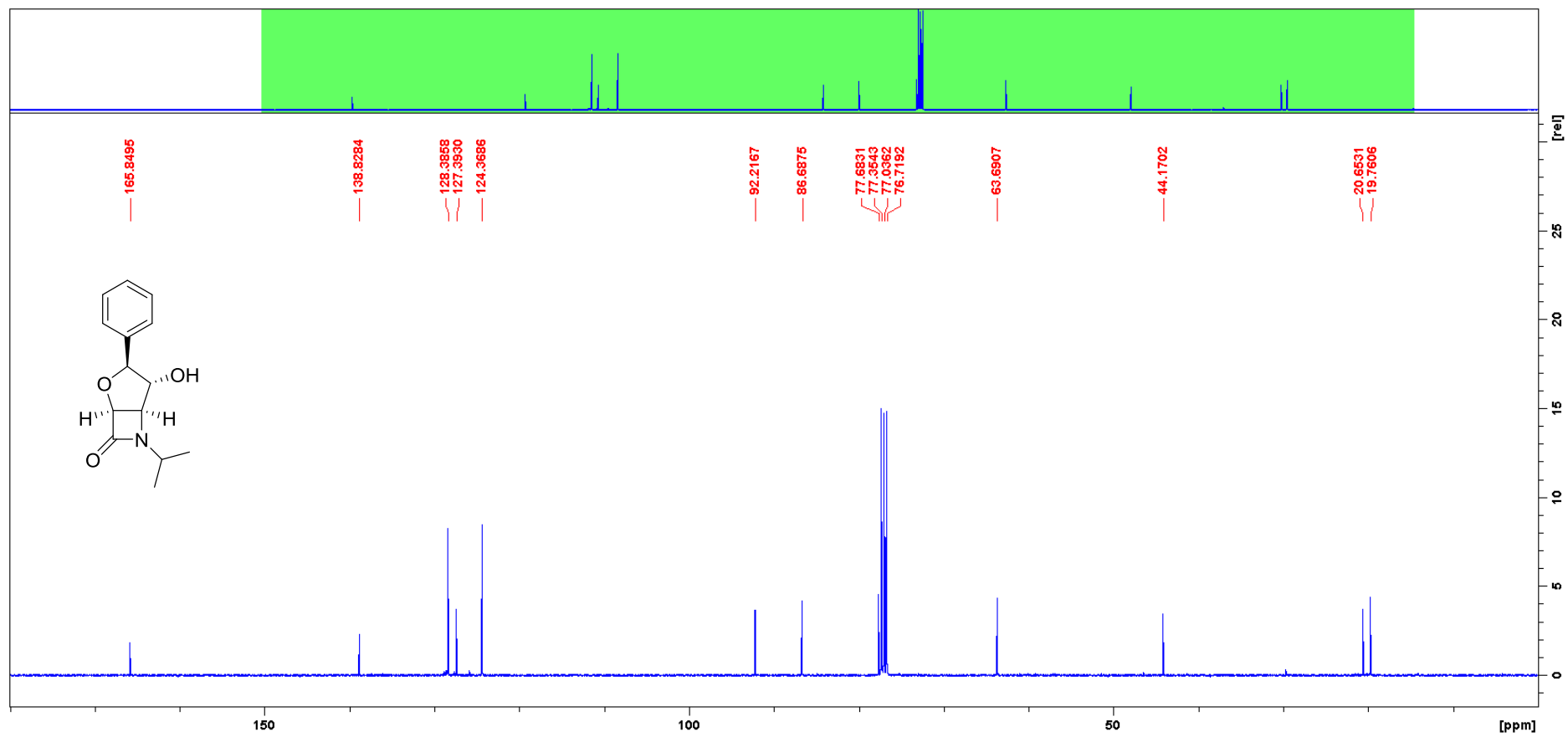


Compound **11a**:  $^1\text{H}$  NMR

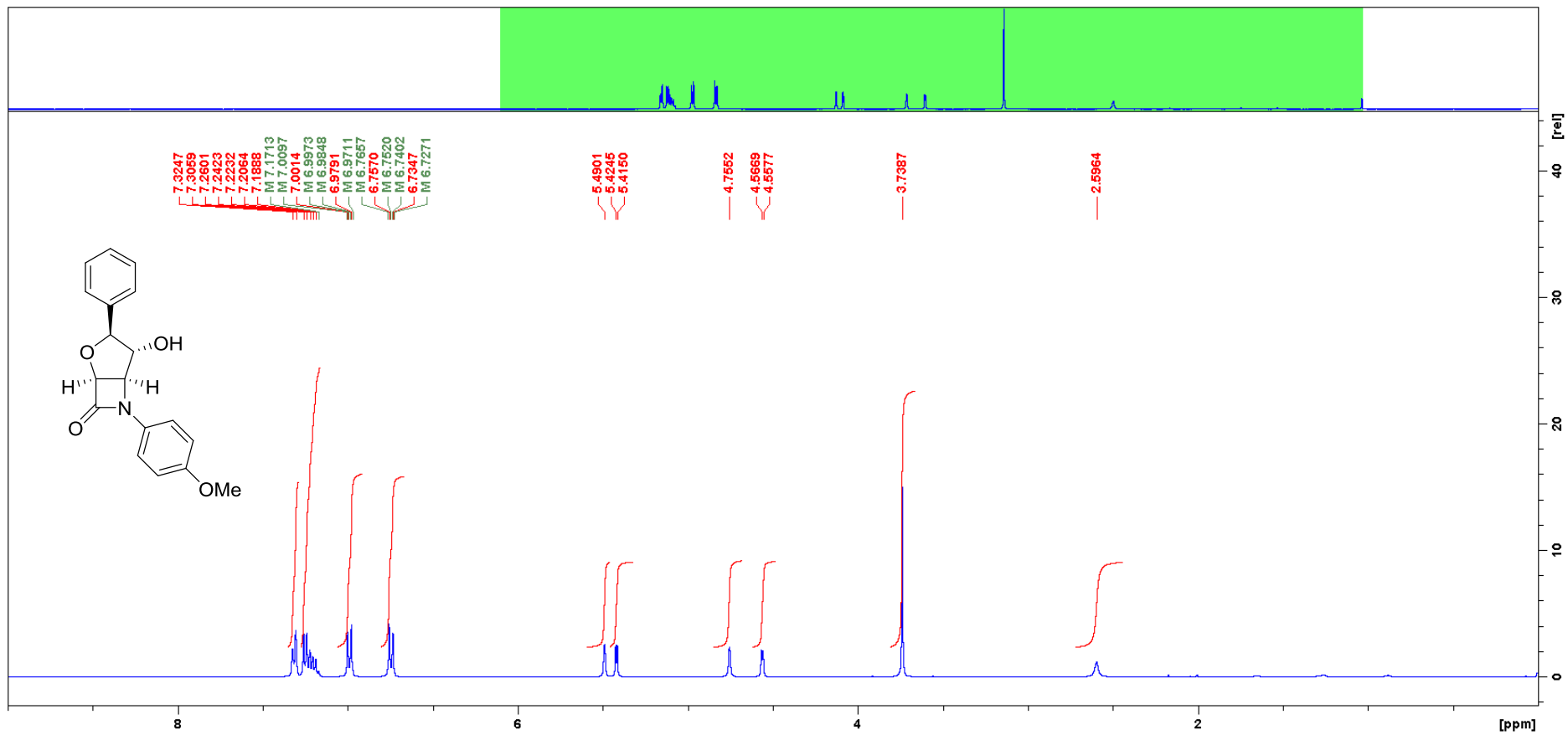




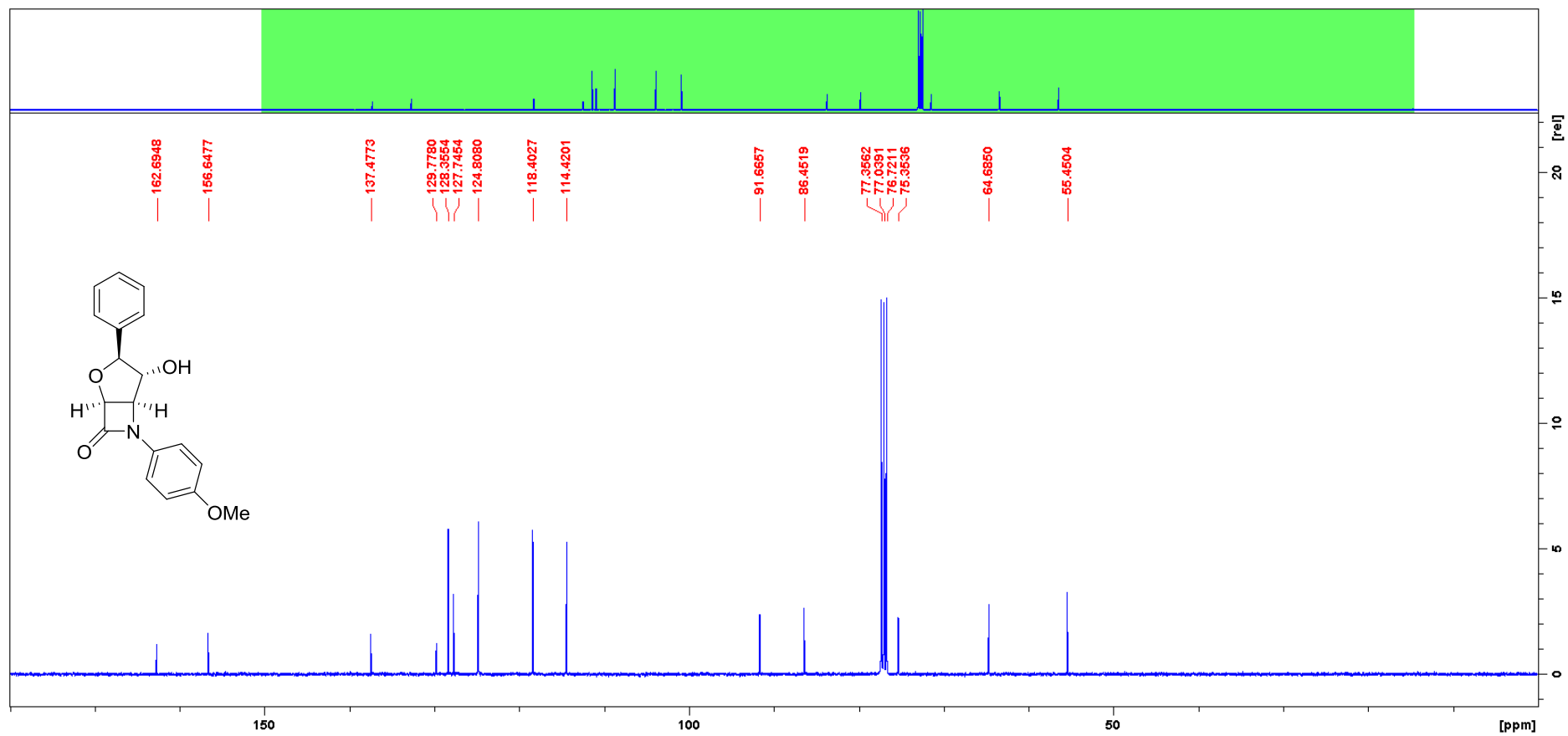
Compound **11a**:  $^{13}\text{C}$  NMR



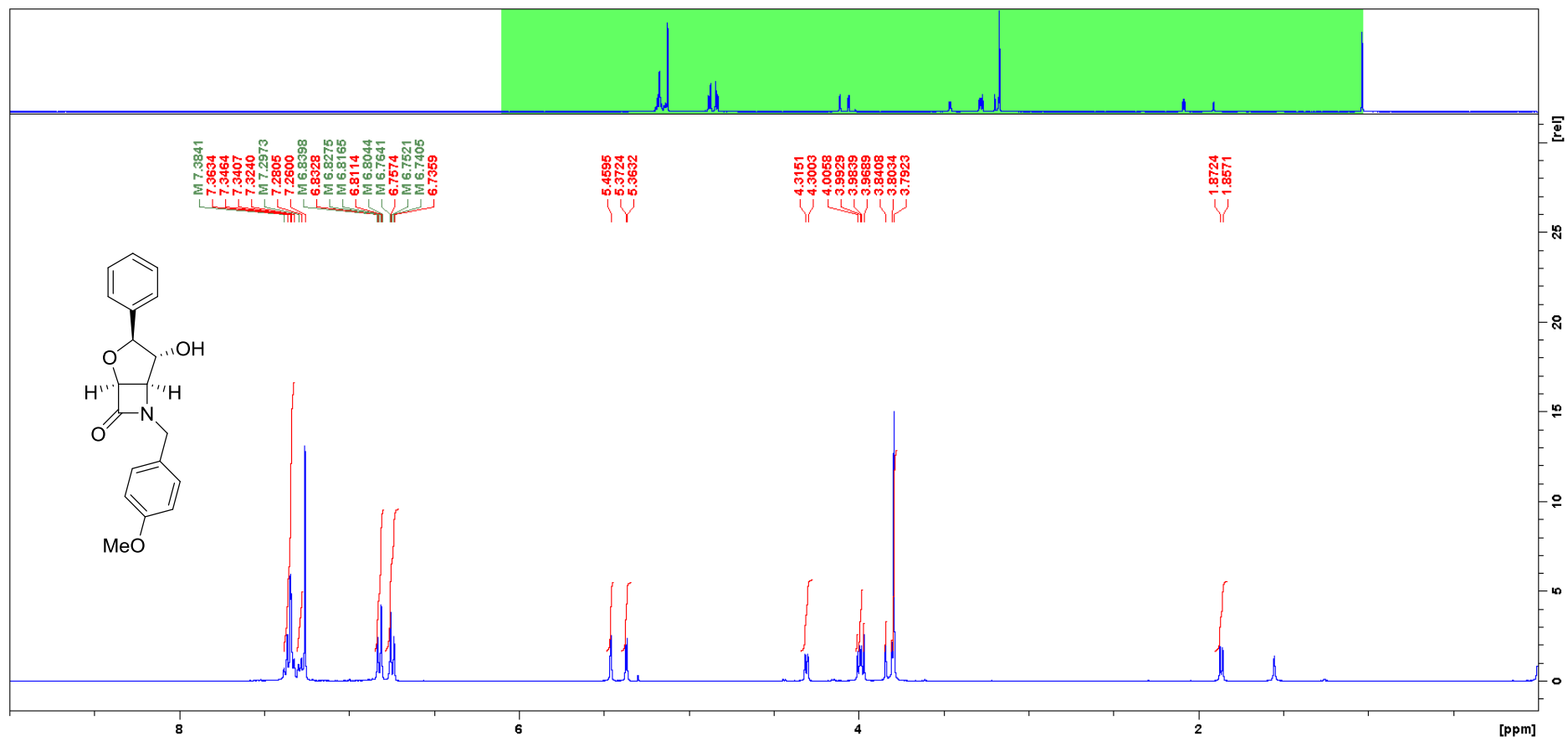
Compound **11b**:  $^1\text{H}$  NMR



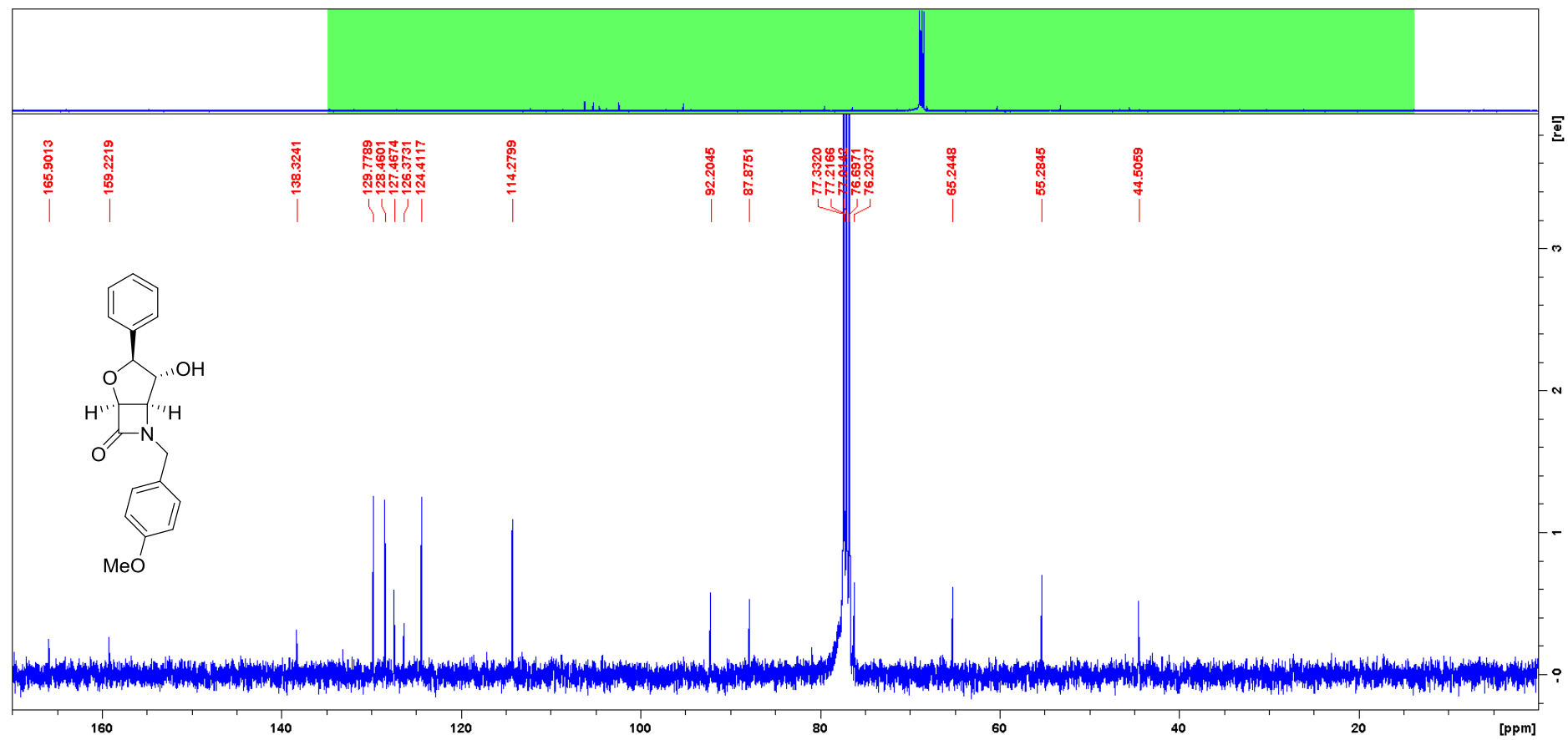
Compound **11b**:  $^{13}\text{C}$  NMR



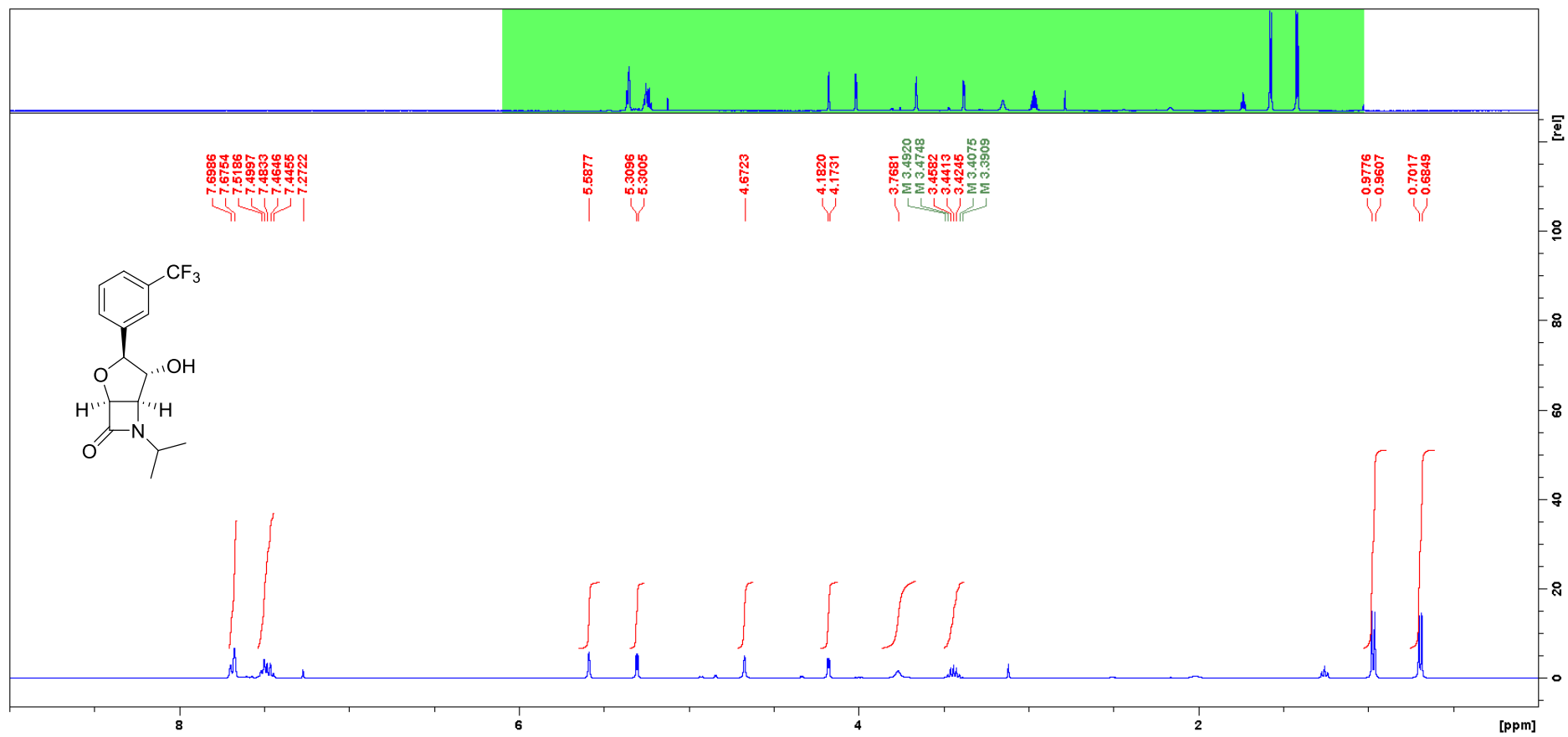
Compound **11c**:  $^1\text{H}$  NMR



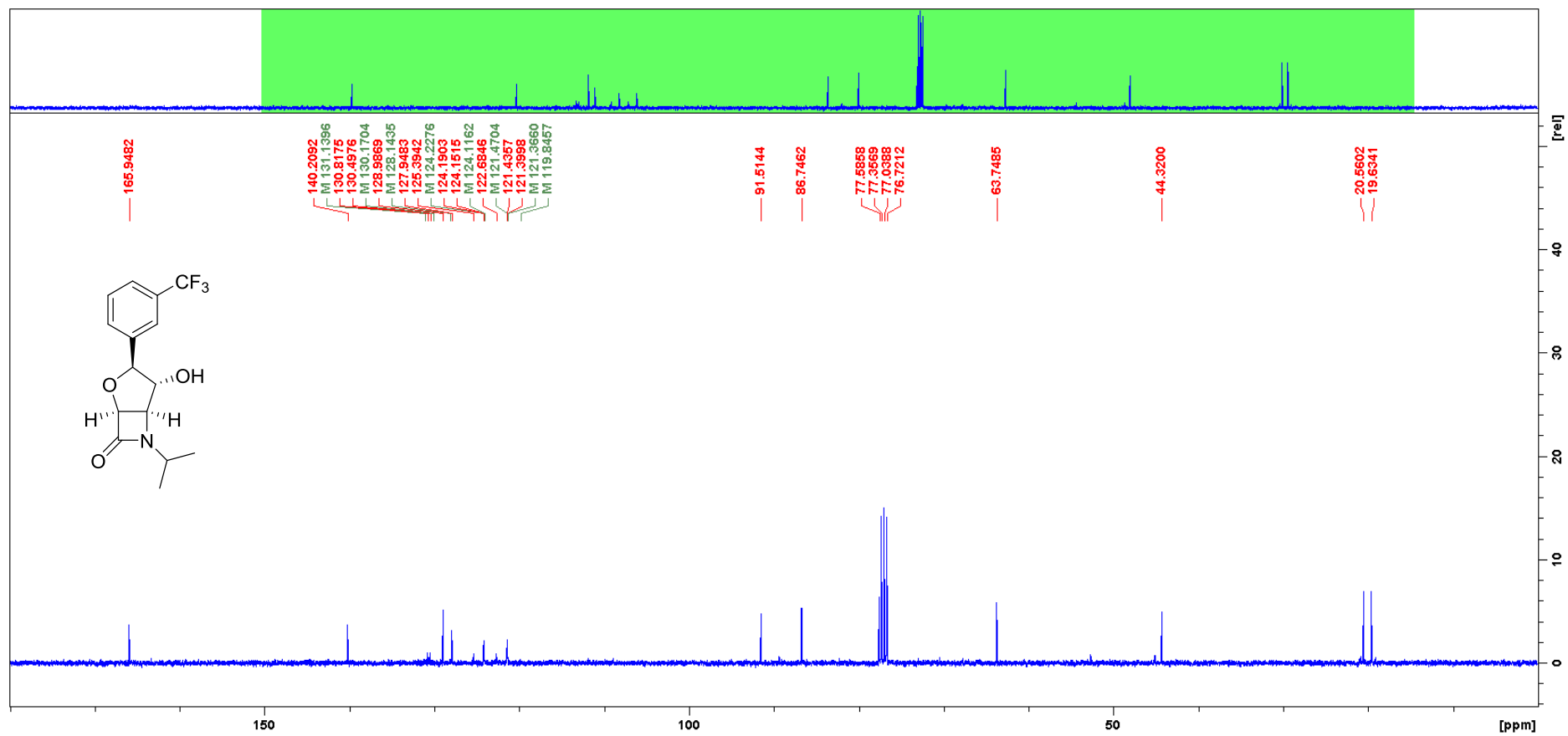
Compound **11c**:  $^{13}\text{C}$  NMR



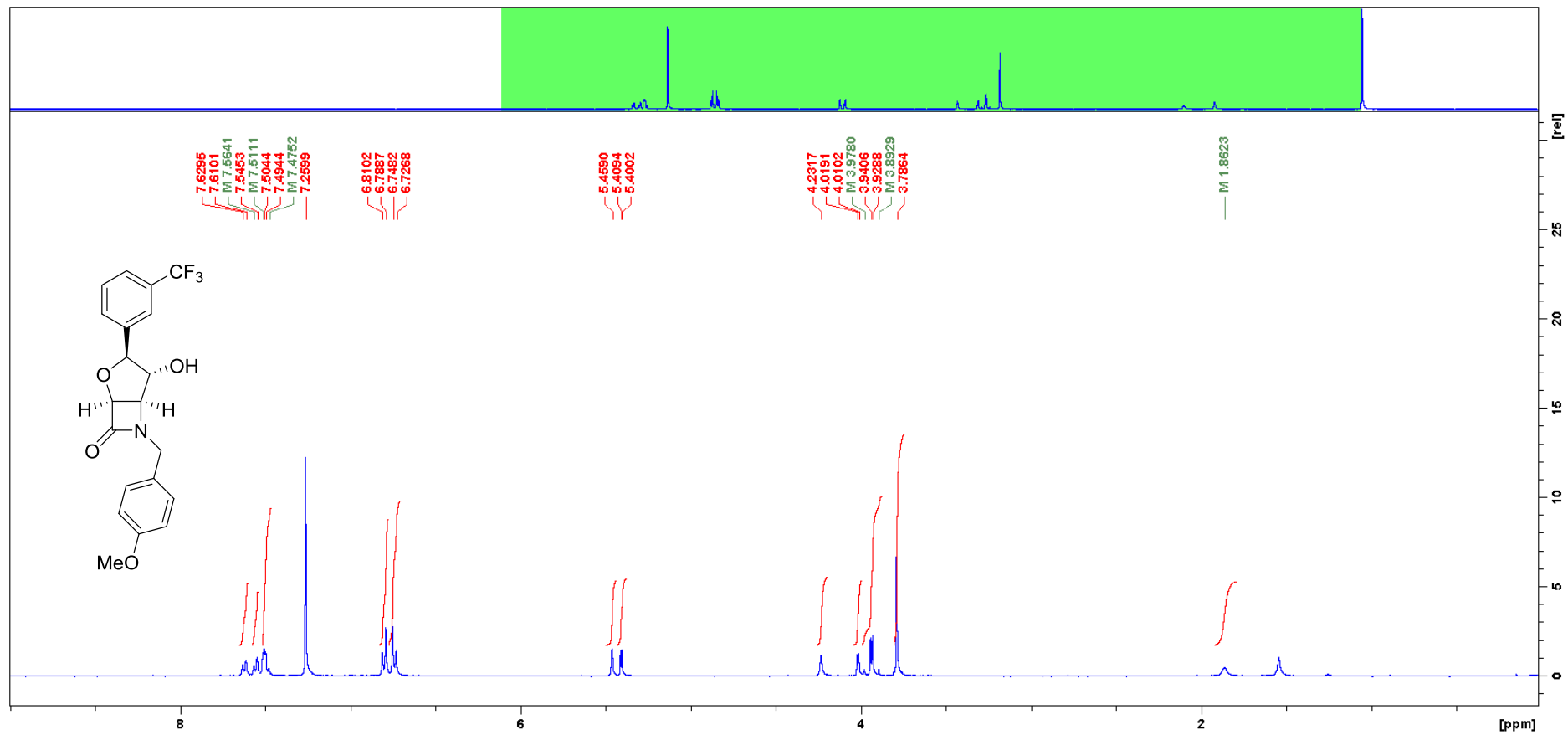
Compound **11d**:  $^1\text{H}$  NMR



Compound **11d**:  $^{13}\text{C}$  NMR

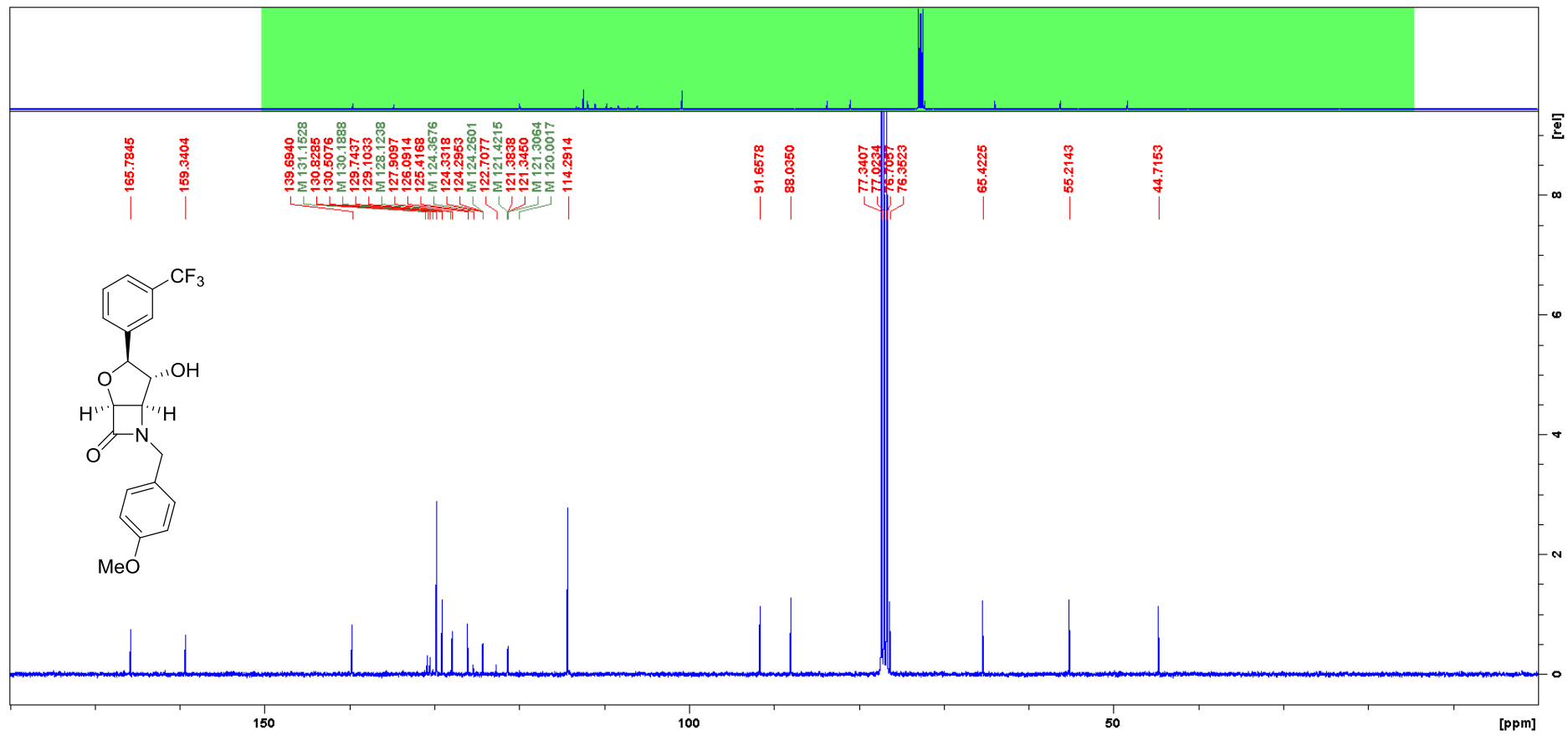


Compound 11e: <sup>1</sup>H NMR

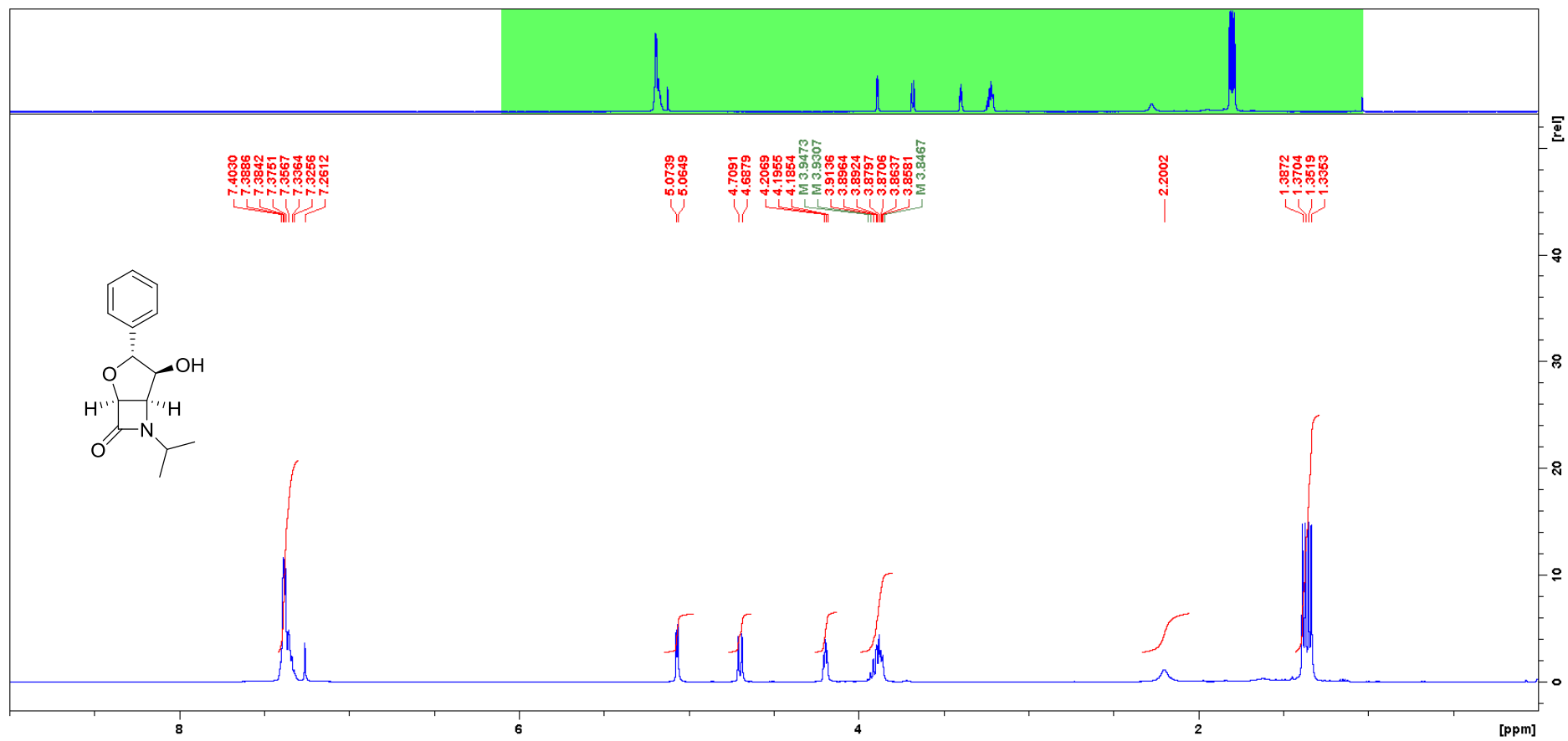




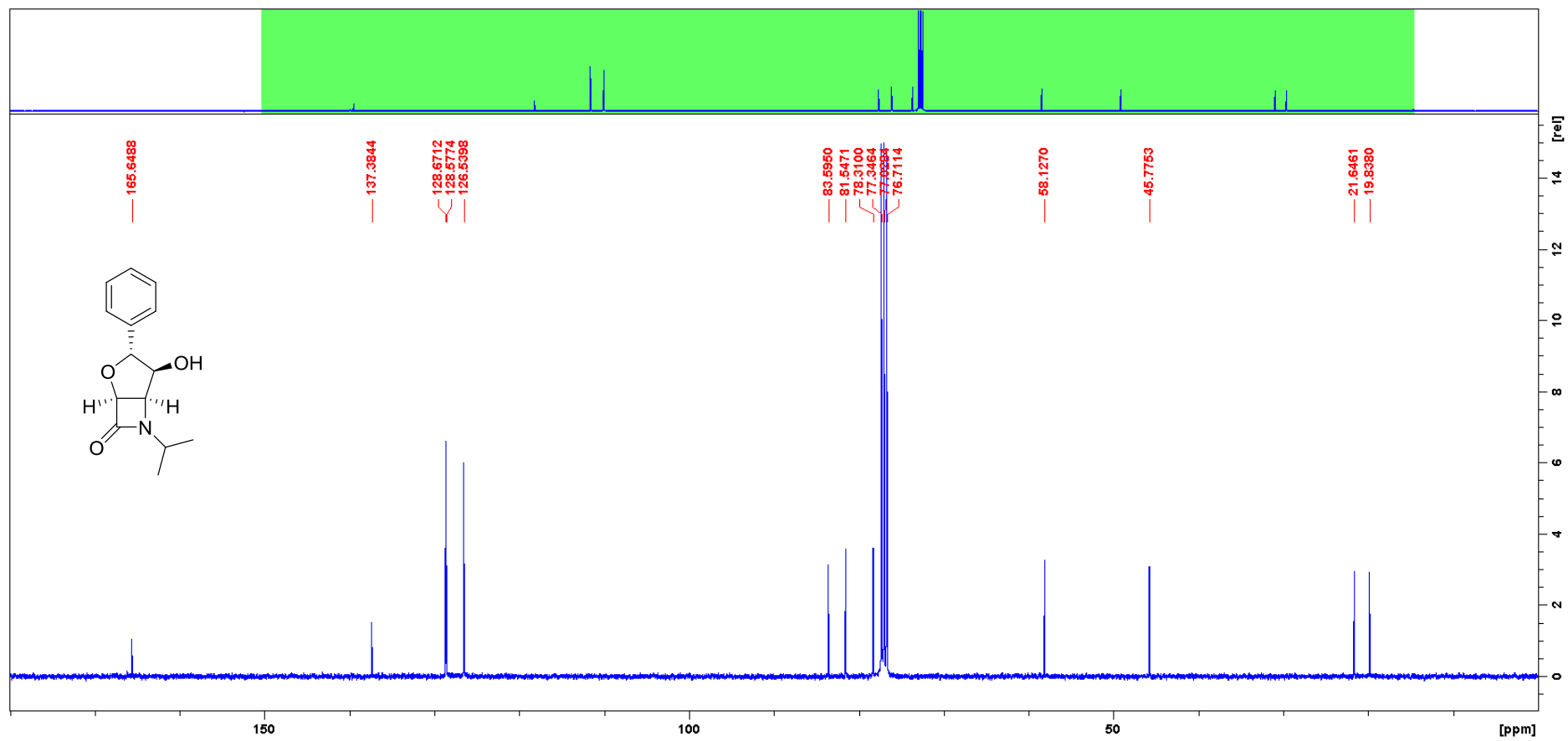
Compound 11e: <sup>13</sup>C NMR



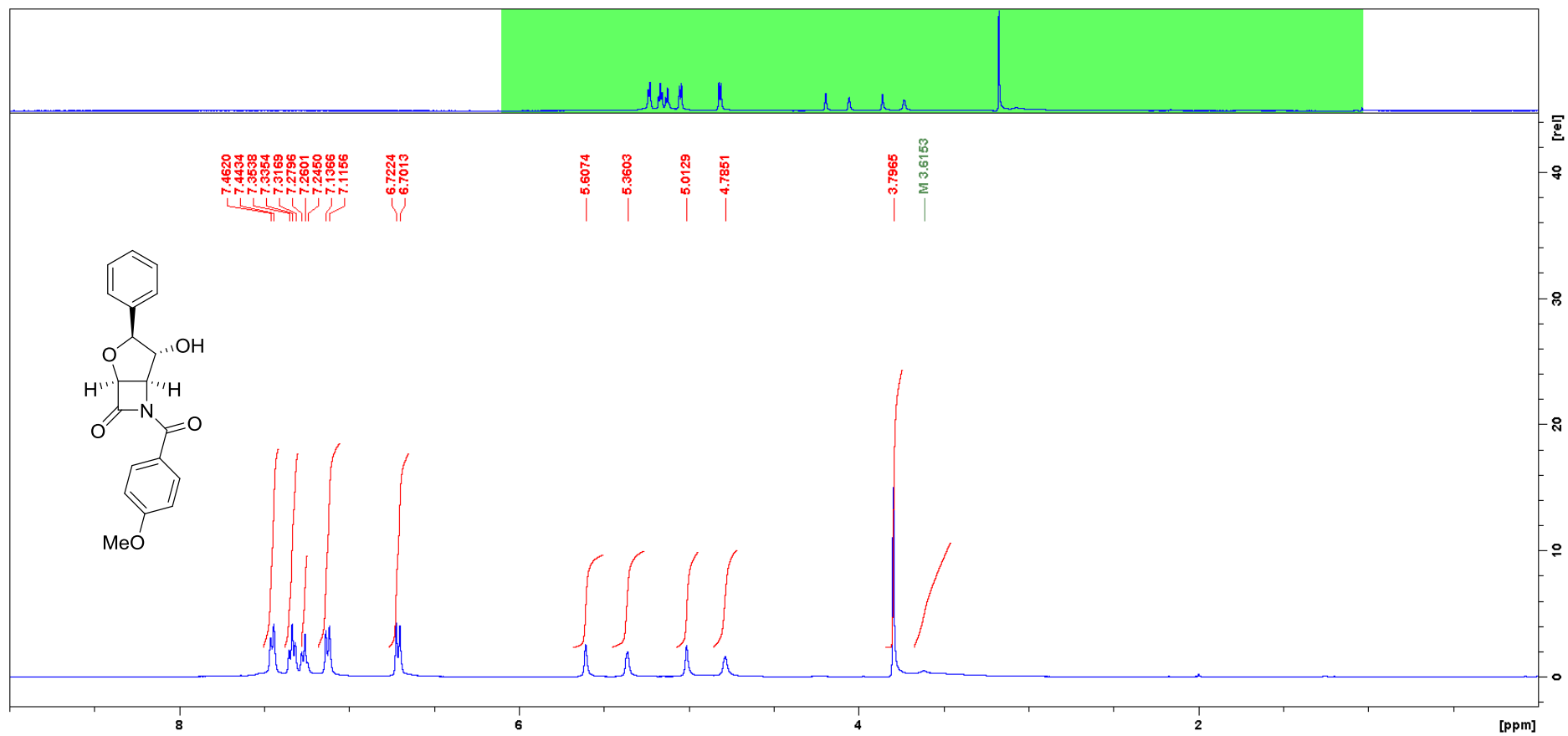
Compound **12a**:  $^1\text{H}$  NMR



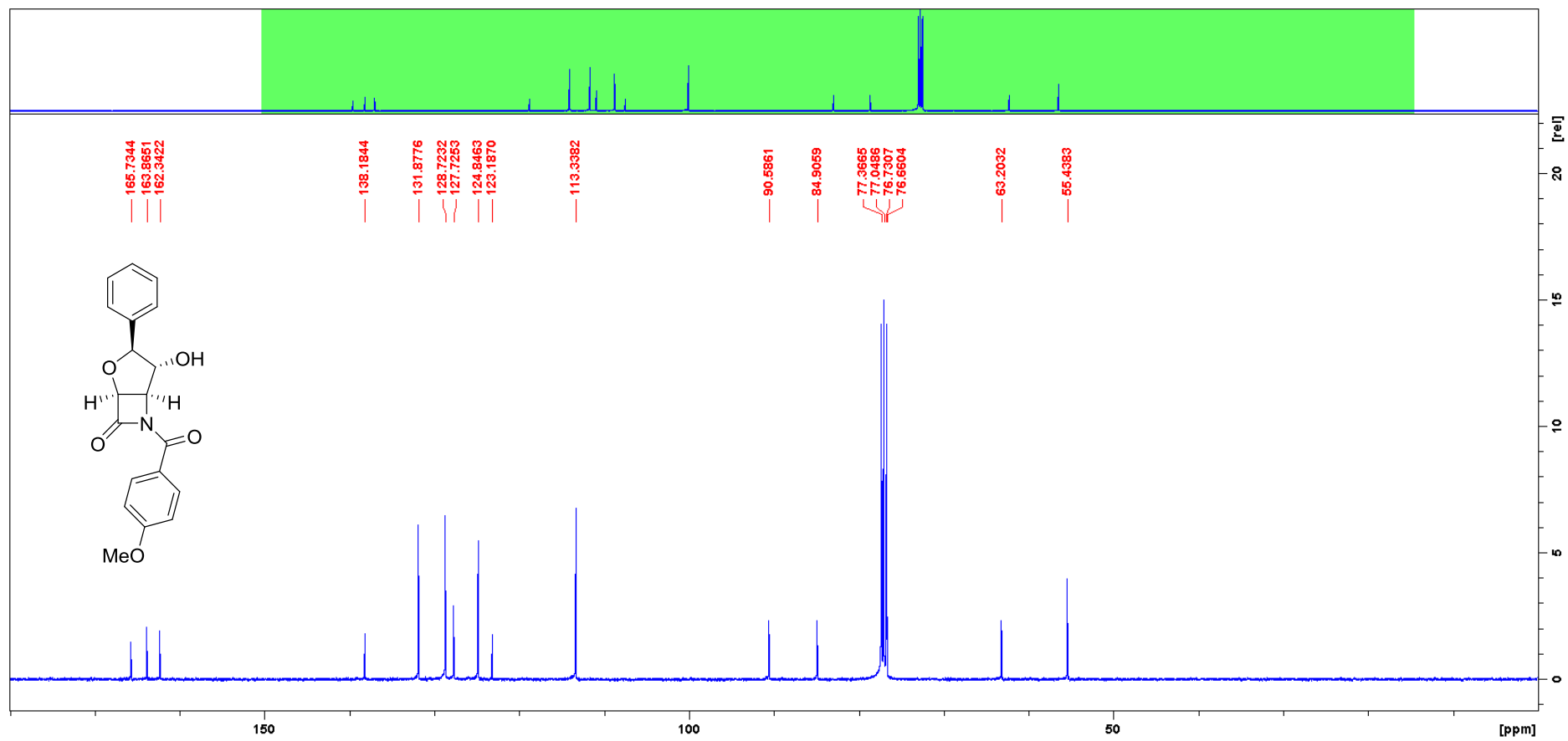
Compound **12a**:  $^{13}\text{C}$  NMR



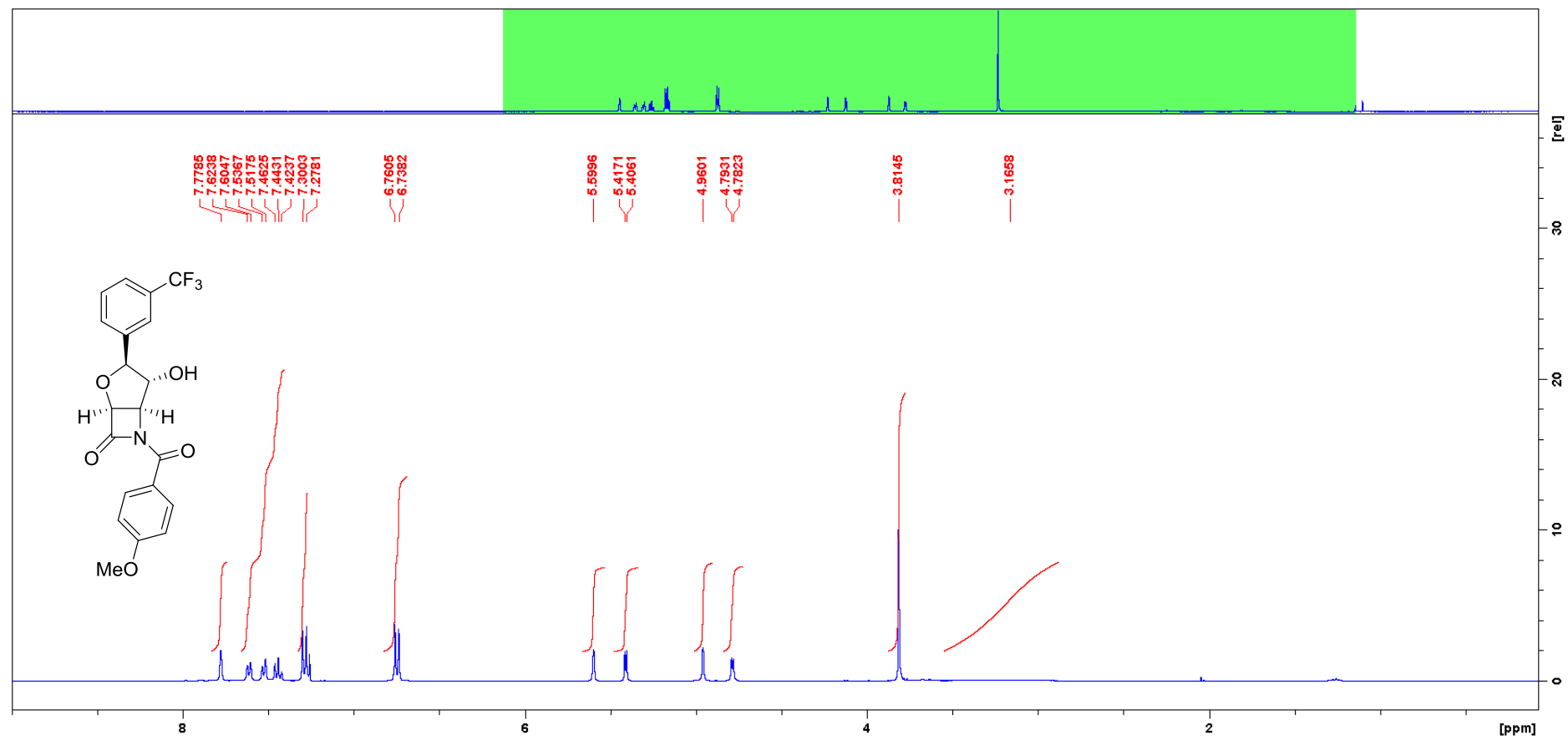
Compound 13a: <sup>1</sup>H NMR



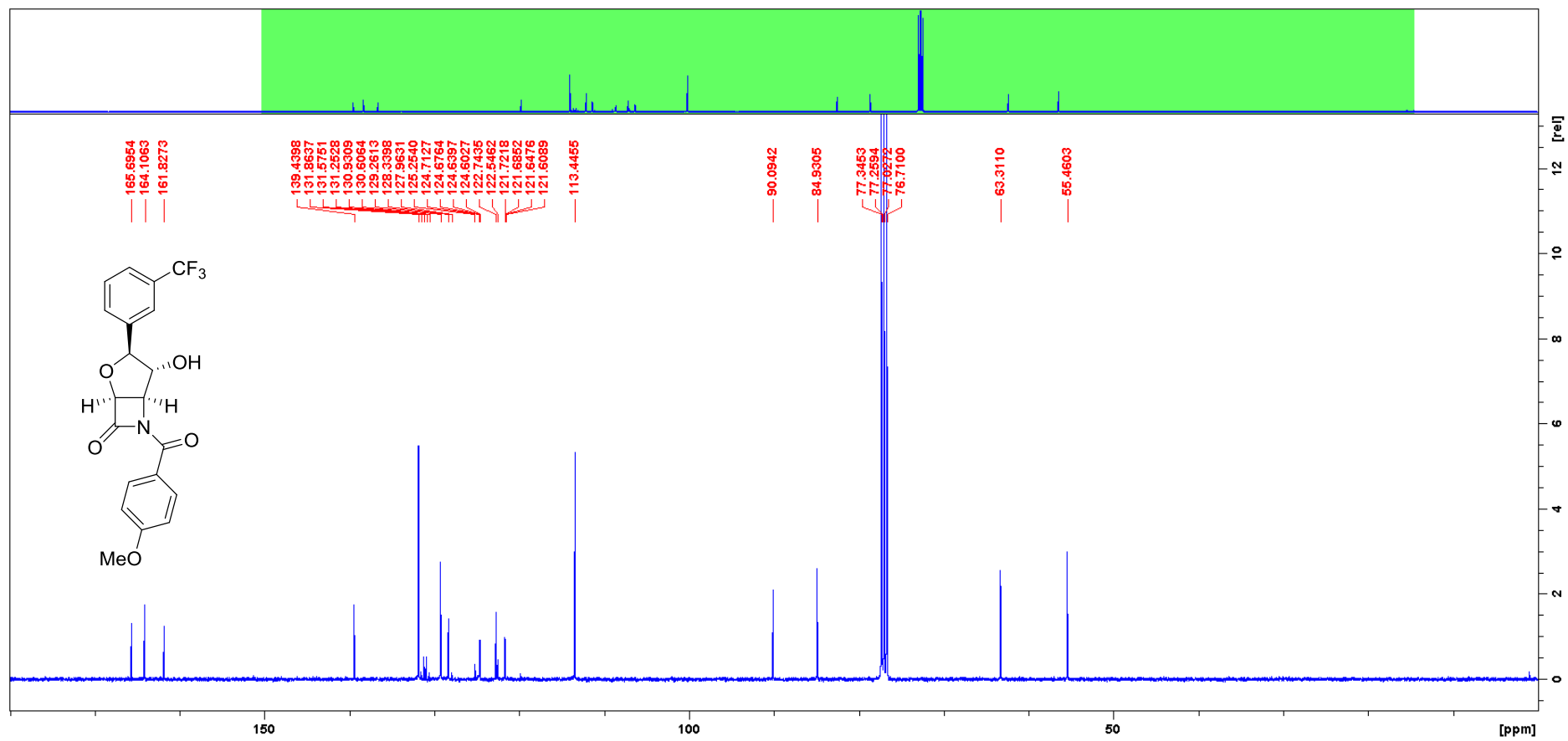
Compound **13a**:  $^{13}\text{C}$  NMR



Compound **13b**:  $^1\text{H}$  NMR



Compound **13b**:  $^{13}\text{C}$  NMR



## Single crystal X-ray diffraction

For the structures of compounds **11b** and **12a**, X-ray intensity data were collected on a Agilent Supernova Dual Source (Cu at zero) diffractometer equipped with an Atlas CCD detector using CuK $\alpha$  radiation ( $\lambda = 1.54178 \text{ \AA}$ ) and  $\omega$  scans. The images were interpreted and integrated with the program CrysAlisPro (Agilent Technologies) [1]. Using Olex2 [2], the structure was solved by direct methods using the ShelXS structure solution program and refined by full-matrix least-squares on  $F^2$  using the ShelXL program package [3]. Non-hydrogen atoms were anisotropically refined and the hydrogen atoms in the riding mode and isotropic temperature factors fixed at 1.2 times  $U(\text{eq})$  of the parent atoms (1.5 times for methyl and hydroxyl groups).

CCDC 1400949-1400950 contain the supplementary crystallographic data for this paper and can be obtained free of charge via [www.ccdc.cam.ac.uk/conts/retrieving.html](http://www.ccdc.cam.ac.uk/conts/retrieving.html) (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44-1223-336033; or [deposit@ccdc.cam.ac.uk](mailto:deposit@ccdc.cam.ac.uk)).

*Crystal data for compound 11b.*  $\text{C}_{18}\text{H}_{17}\text{NO}_4$ ,  $M = 311.33$ , triclinic, space group  $P-1$  (No. 2),  $a = 6.7690(4) \text{ \AA}$ ,  $b = 17.4058(7) \text{ \AA}$ ,  $c = 26.8238(9) \text{ \AA}$ ,  $\alpha = 94.767(3)^\circ$ ,  $\beta = 94.714(4)^\circ$ ,  $\gamma = 99.371(4)^\circ$ ,  $V = 3092.7(2) \text{ \AA}^3$ ,  $Z = 8$ ,  $T = 100 \text{ K}$ ,  $\rho_{\text{calc}} = 1.337 \text{ g cm}^{-3}$ ,  $\mu(\text{Cu-K}\alpha) = 0.781 \text{ mm}^{-1}$ ,  $F(000) = 1312$ , 28410 reflections measured, 12222 unique ( $R_{\text{int}} = 0.0660$ ) which were used in all calculations. The final  $R1$  was 0.0617 ( $I > 2\sigma(I)$ ) and  $wR2$  was 0.1754 (all data). The asymmetric unit contains four crystallographic independent molecules.

*Crystal data for compound 12a.*  $\text{C}_{14}\text{H}_{17}\text{NO}_3$ ,  $M = 247.29$ , orthorhombic, space group  $Pna2_1$  (No. 33),  $a = 16.3439(5) \text{ \AA}$ ,  $b = 5.9484(2) \text{ \AA}$ ,  $c = 12.9762(5) \text{ \AA}$ ,  $V = 1261.55(8) \text{ \AA}^3$ ,  $Z = 4$ ,  $T = 100 \text{ K}$ ,  $\rho_{\text{calc}} = 1.302 \text{ g cm}^{-3}$ ,  $\mu(\text{Cu-K}\alpha) = 0.747 \text{ mm}^{-1}$ ,  $F(000) = 528$ , 6703 reflections measured, 2069 unique ( $R_{\text{int}} = 0.0391$ ) which were used in all calculations. The final  $R1$  was 0.0326 ( $I > 2\sigma(I)$ ) and  $wR2$  was 0.0820 (all data). The crystal appeared to be racemically twinned, hence the structure shows a refined Flack parameter of 0.49(18).

[1] Agilent (2013). CrysAlis PRO. Agilent Technologies UK Ltd, Yarnton, England.

[2] O.V. Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard & H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Cryst.* (2009). 42, 339-341.

[3] SHELXS, G.M. Sheldrick, *Acta Cryst.* (2008). A64, 112-122.