

Supporting Information for:

# Hypervalent Iodonium Alkynyl Triflate Generated Phenylcyanocarbene and Its Reactivity with Aromatic Systems

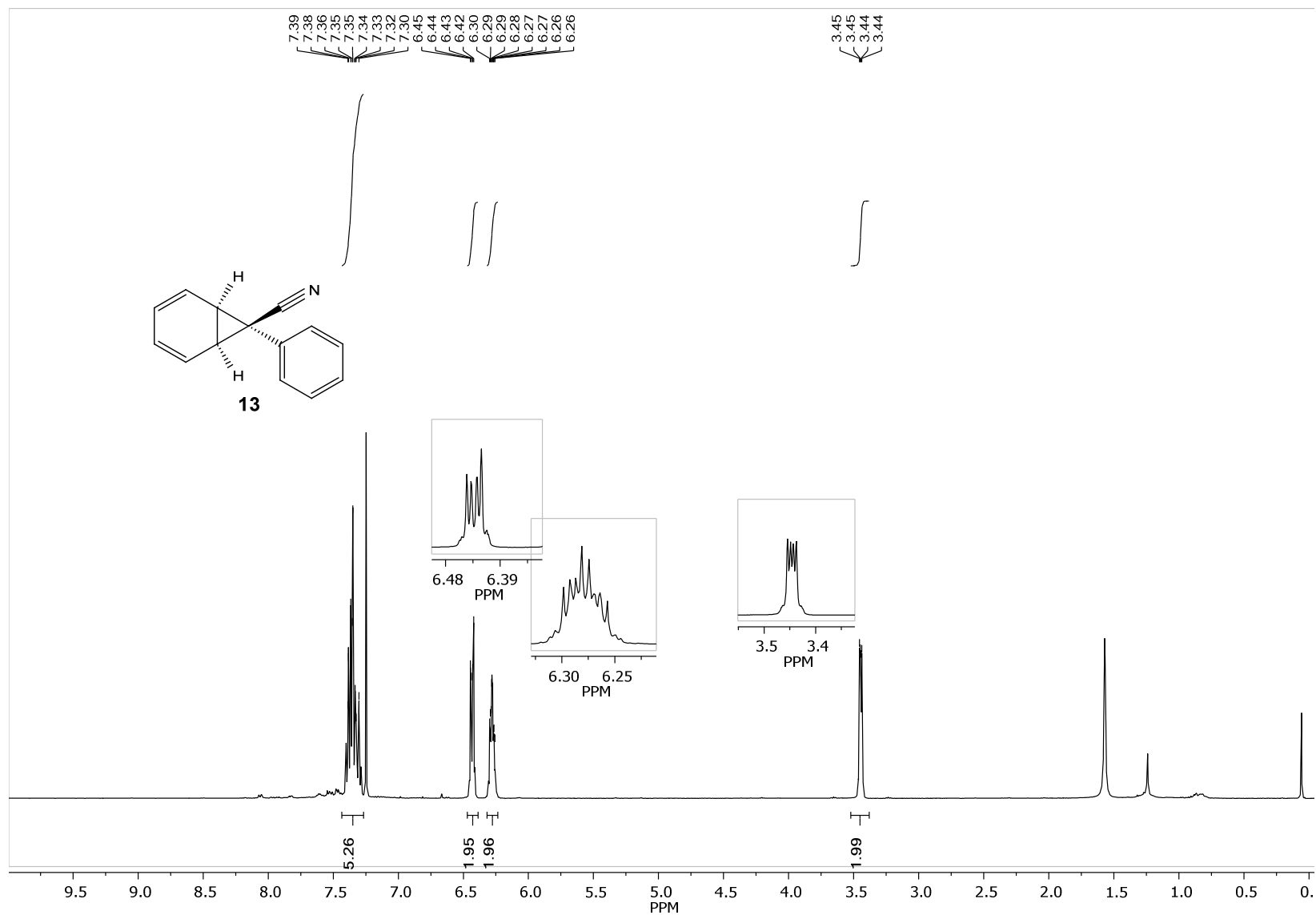
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<sup>†</sup>Department of Chemistry and Biochemistry, University of North Carolina at Greensboro, 435 Sullivan Science Building, Greensboro, North Carolina 27402, United States

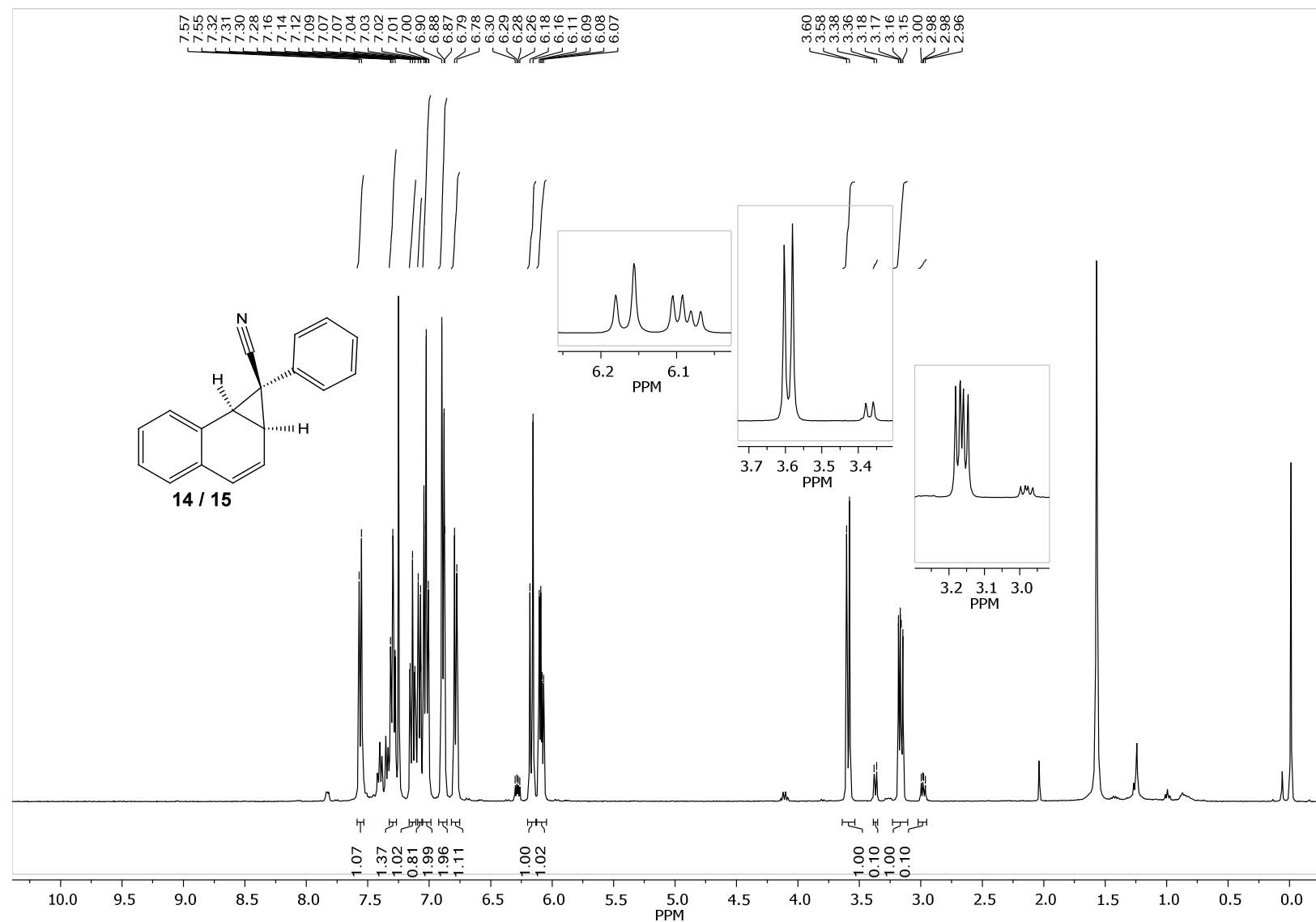
<sup>‡</sup>Department of Chemistry, Adelphi University, 1 South Avenue, Garden City, New York 11530, United States

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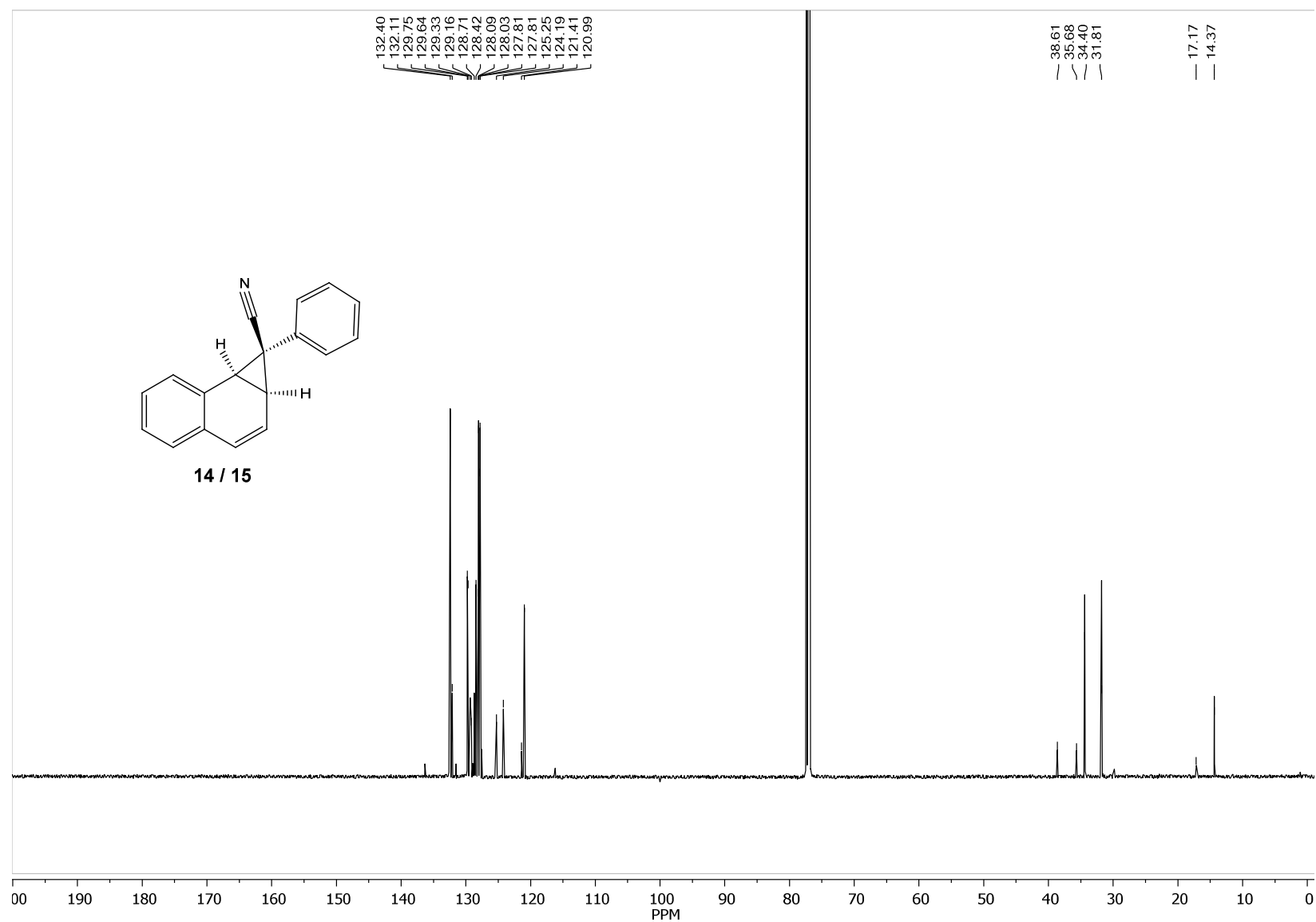
<sup>1</sup>H NMR for compound **13**



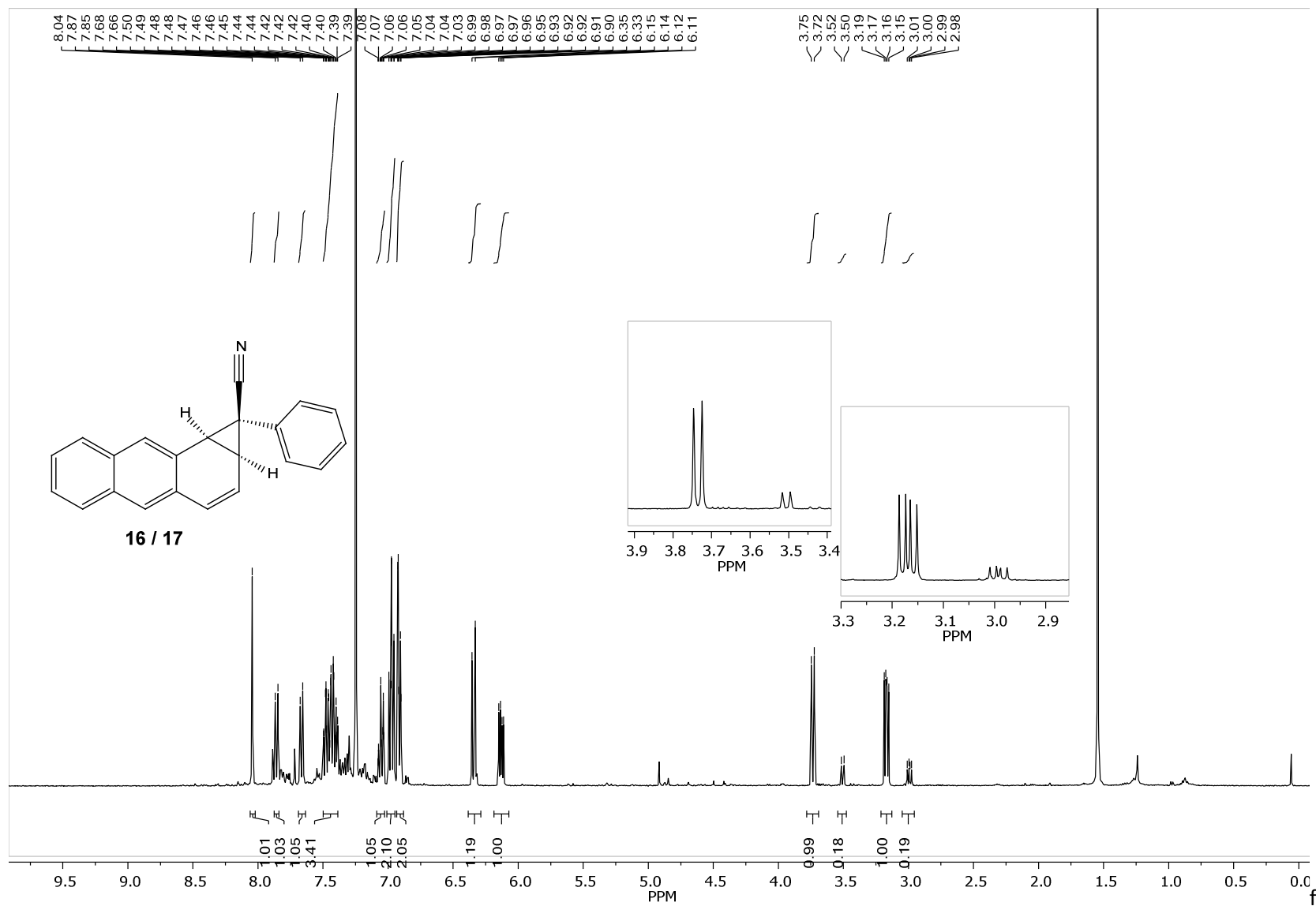
<sup>1</sup>H NMR for compounds **14/15**



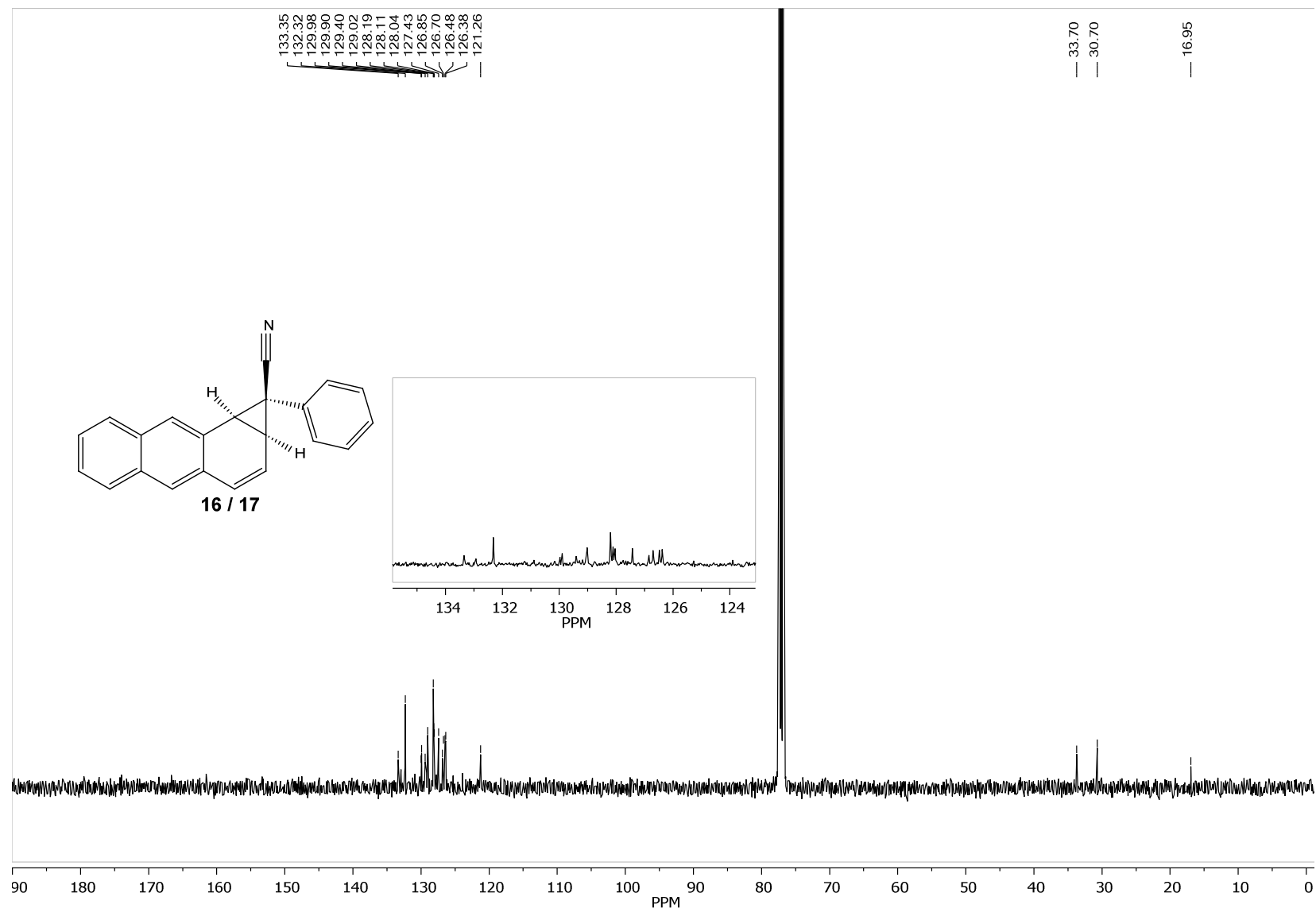
<sup>13</sup>C NMR for compounds **14/15**



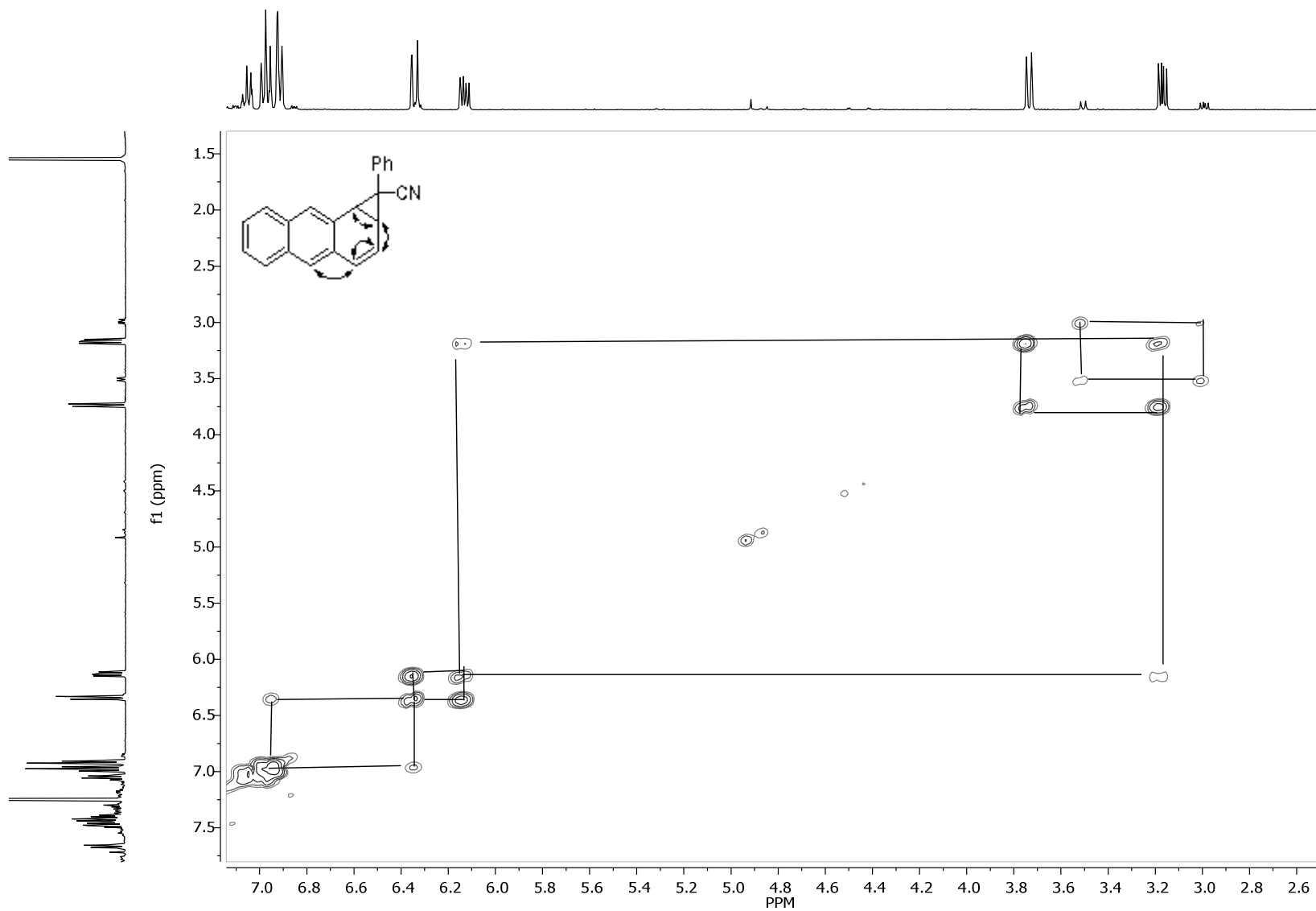
<sup>1</sup>H NMR for compounds **16/17**



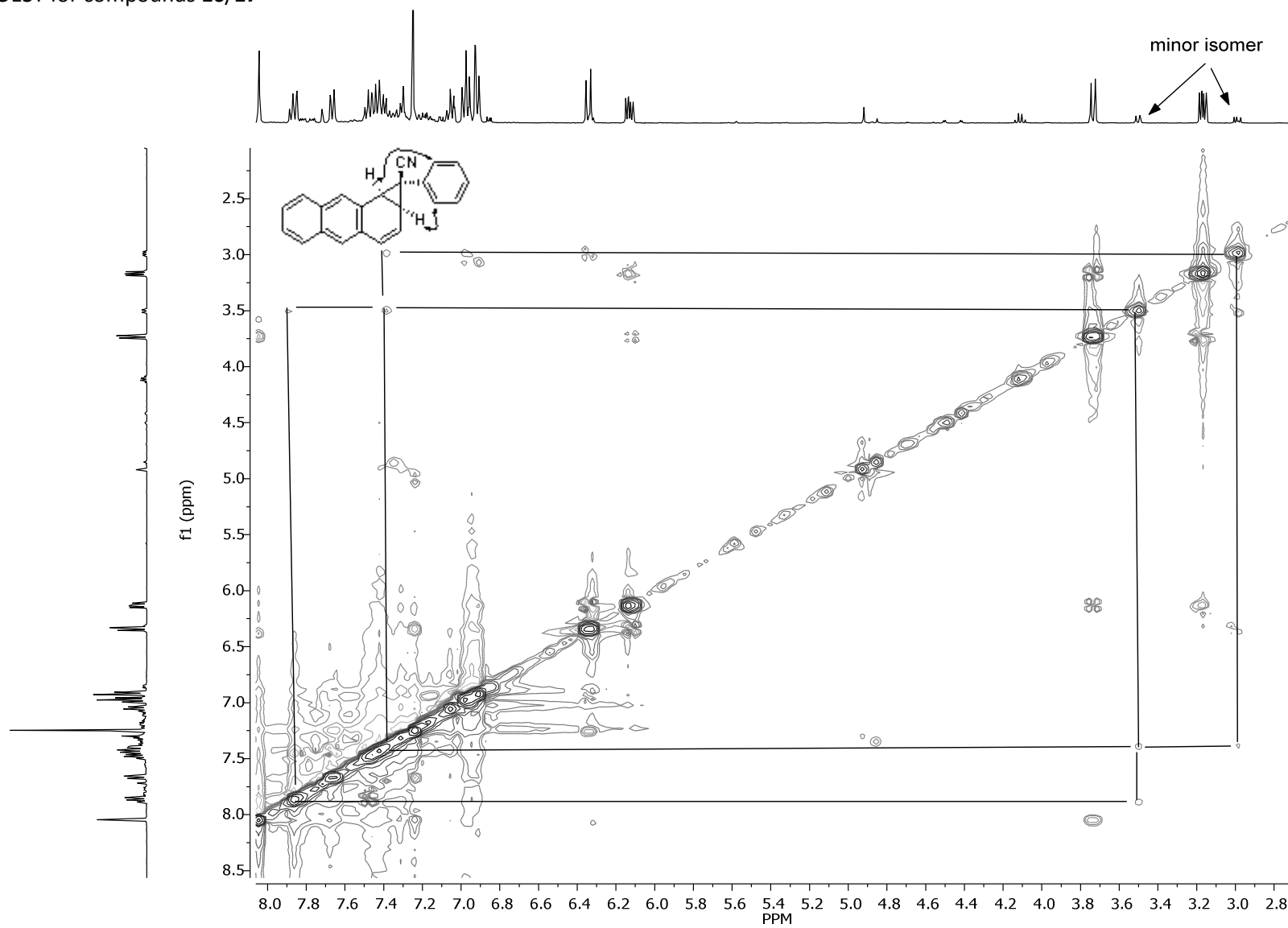
<sup>13</sup>C NMR for compounds **16/17**



$^1\text{H}$ - $^1\text{H}$  COSY for compounds **16/17**

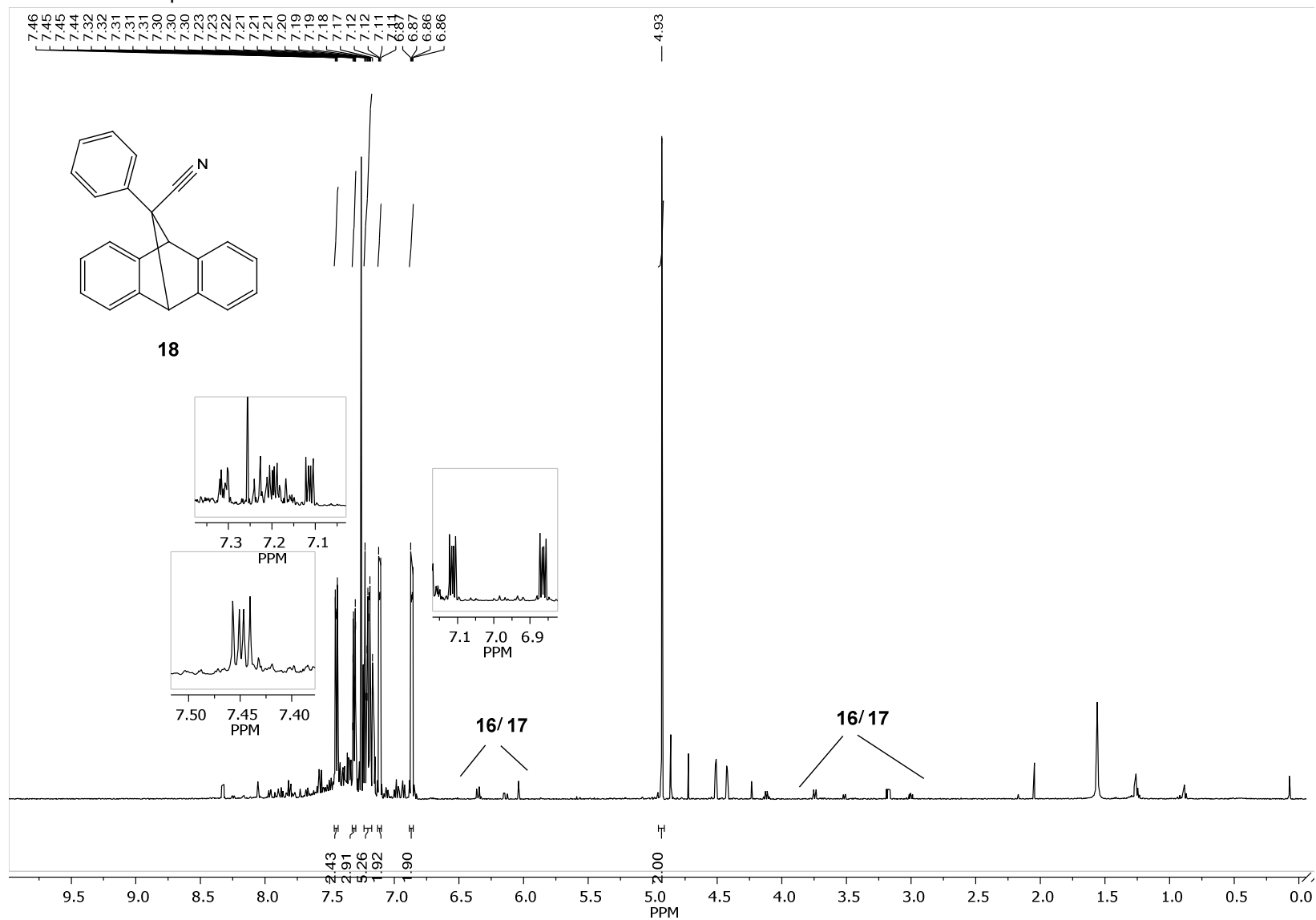


NOESY for compounds **16/17**

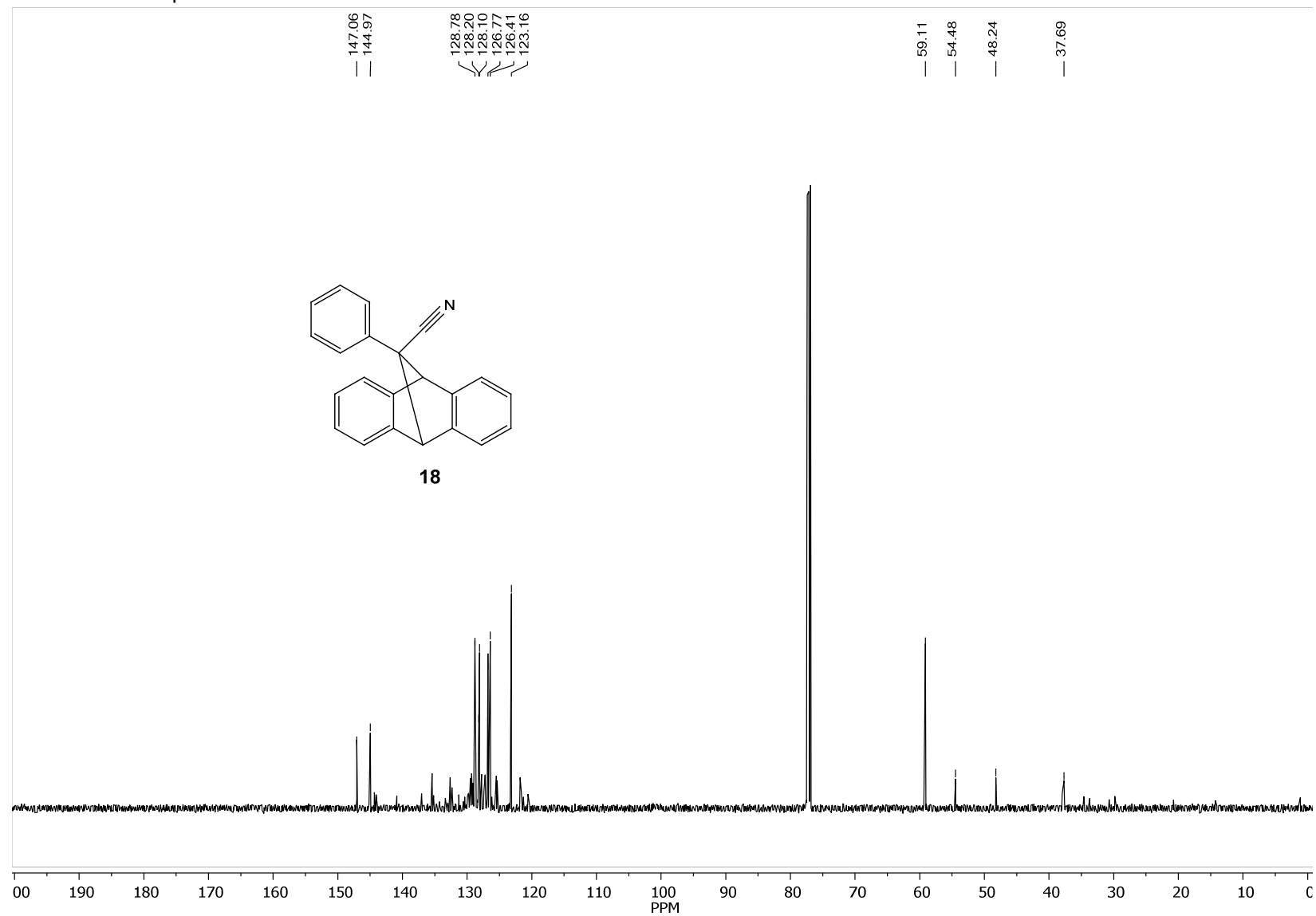




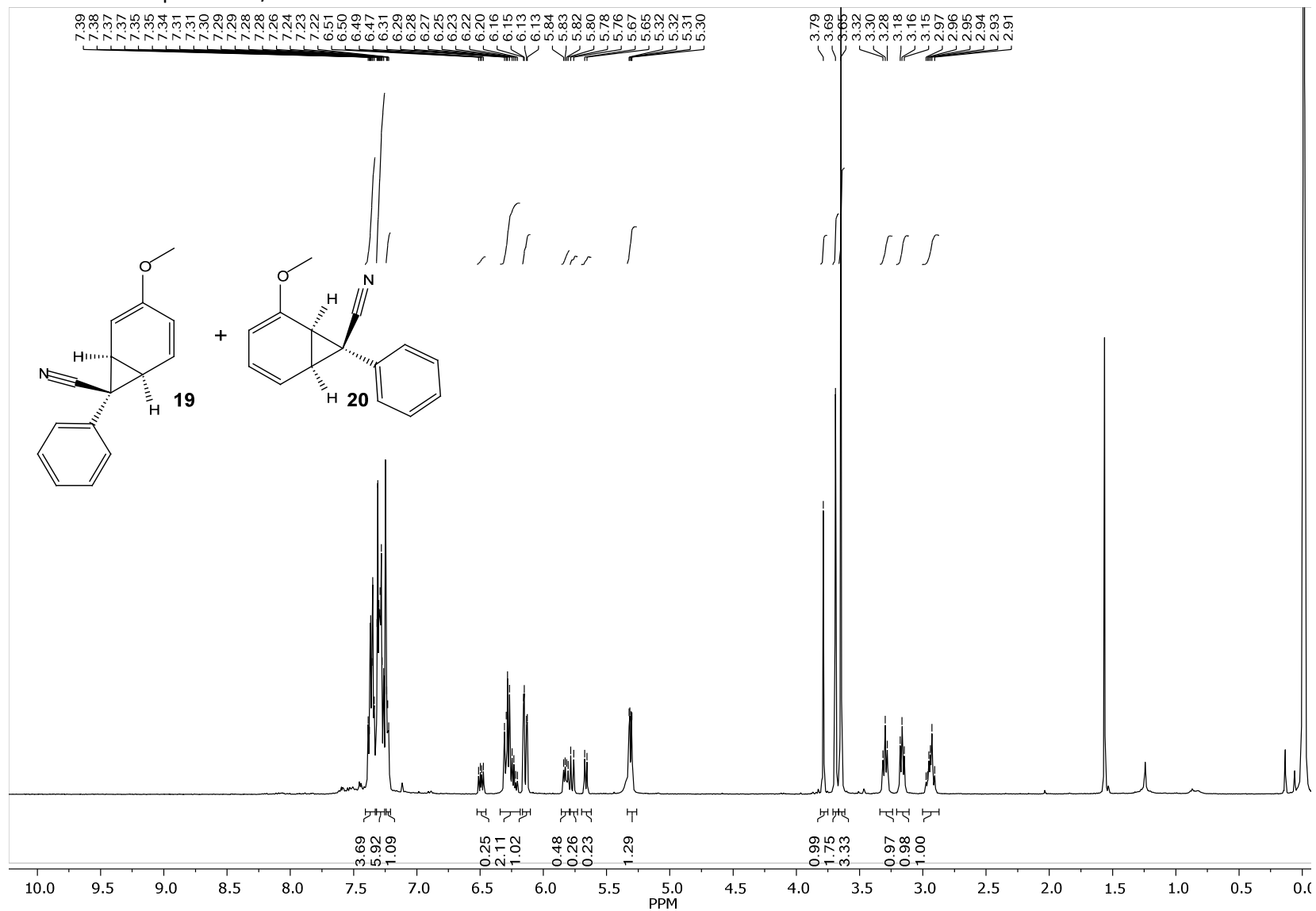
<sup>1</sup>H NMR for compound **18**



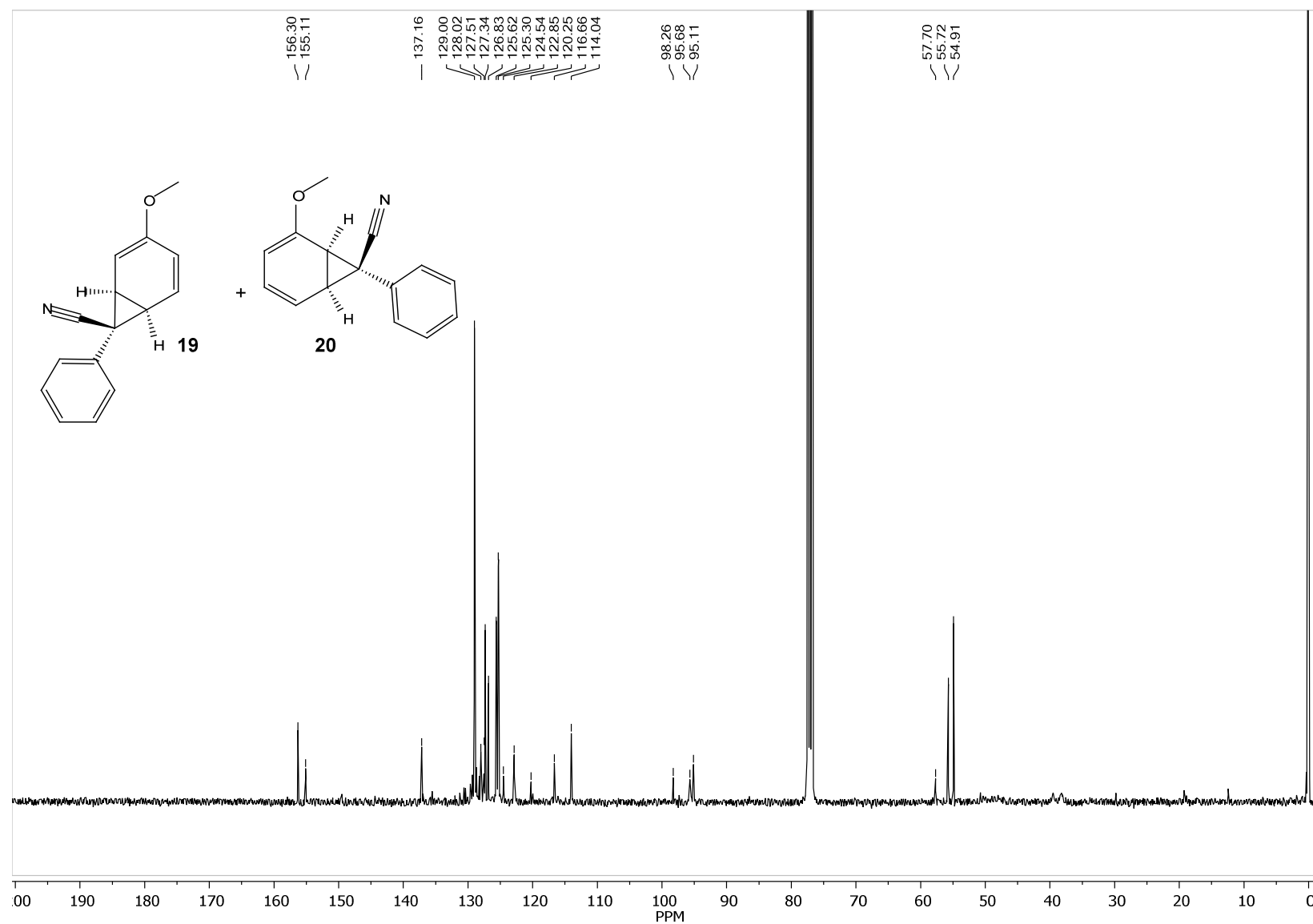
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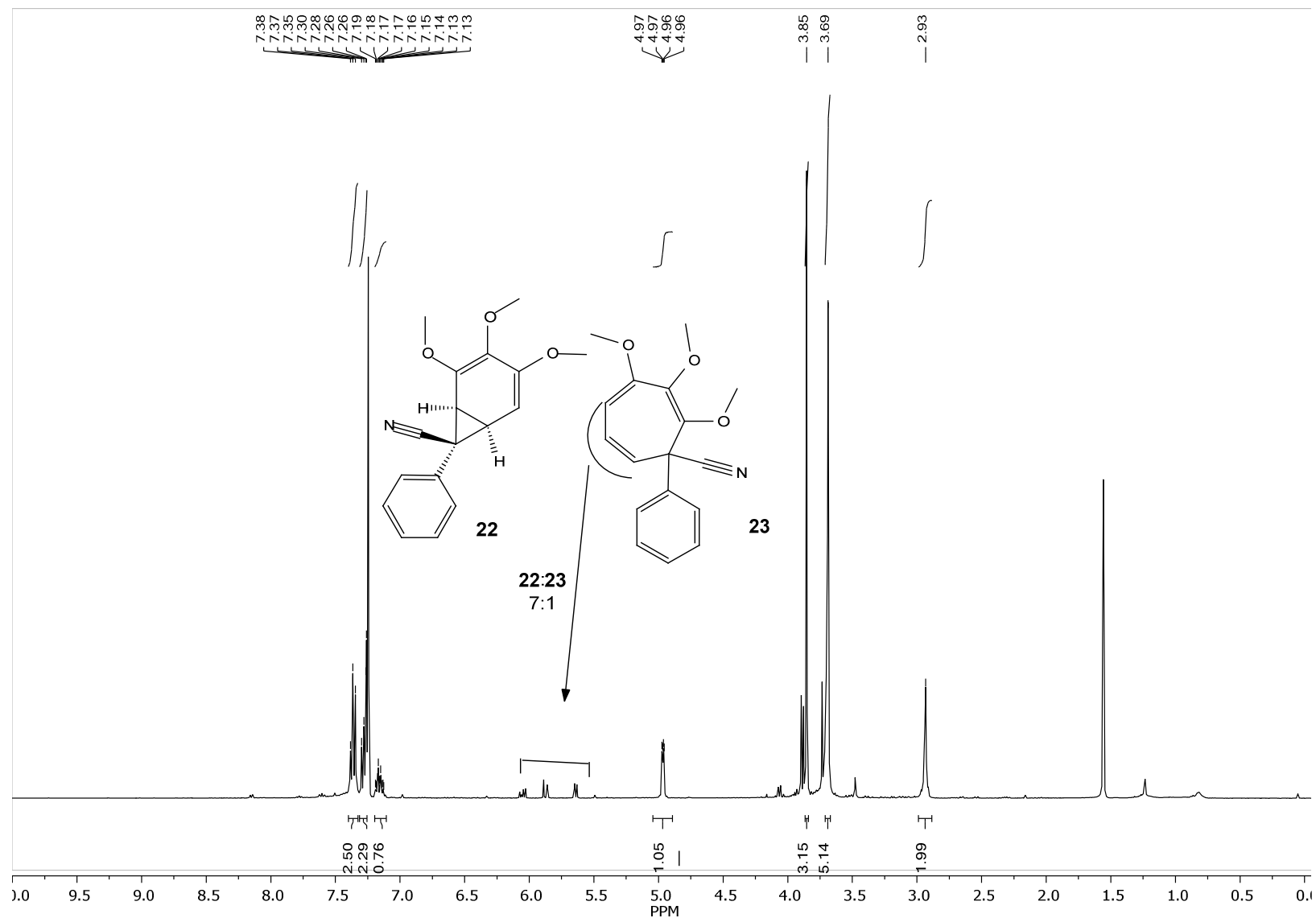
<sup>1</sup>H NMR for compounds **19/20**



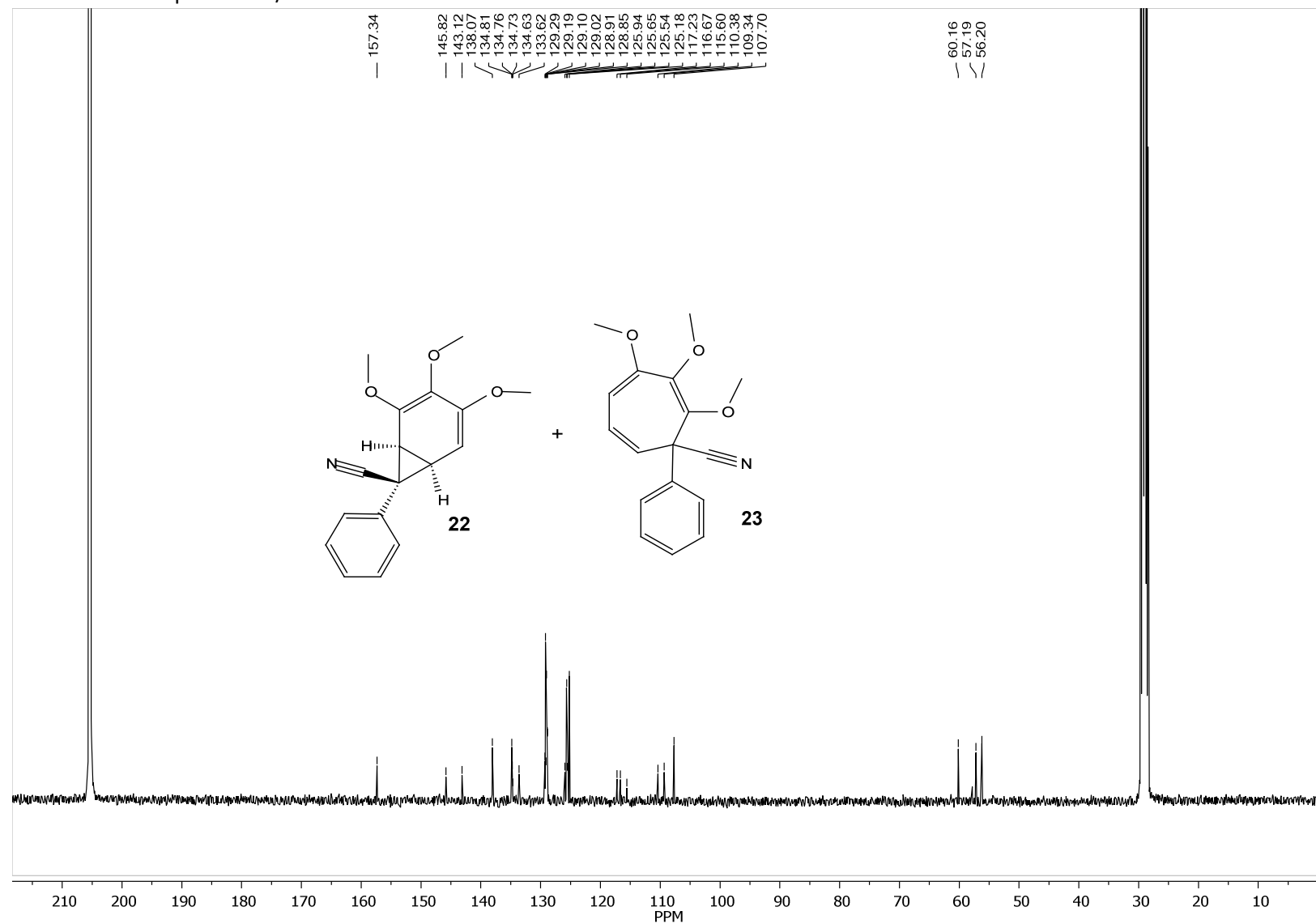
<sup>13</sup>C NMR for compounds **19/20**



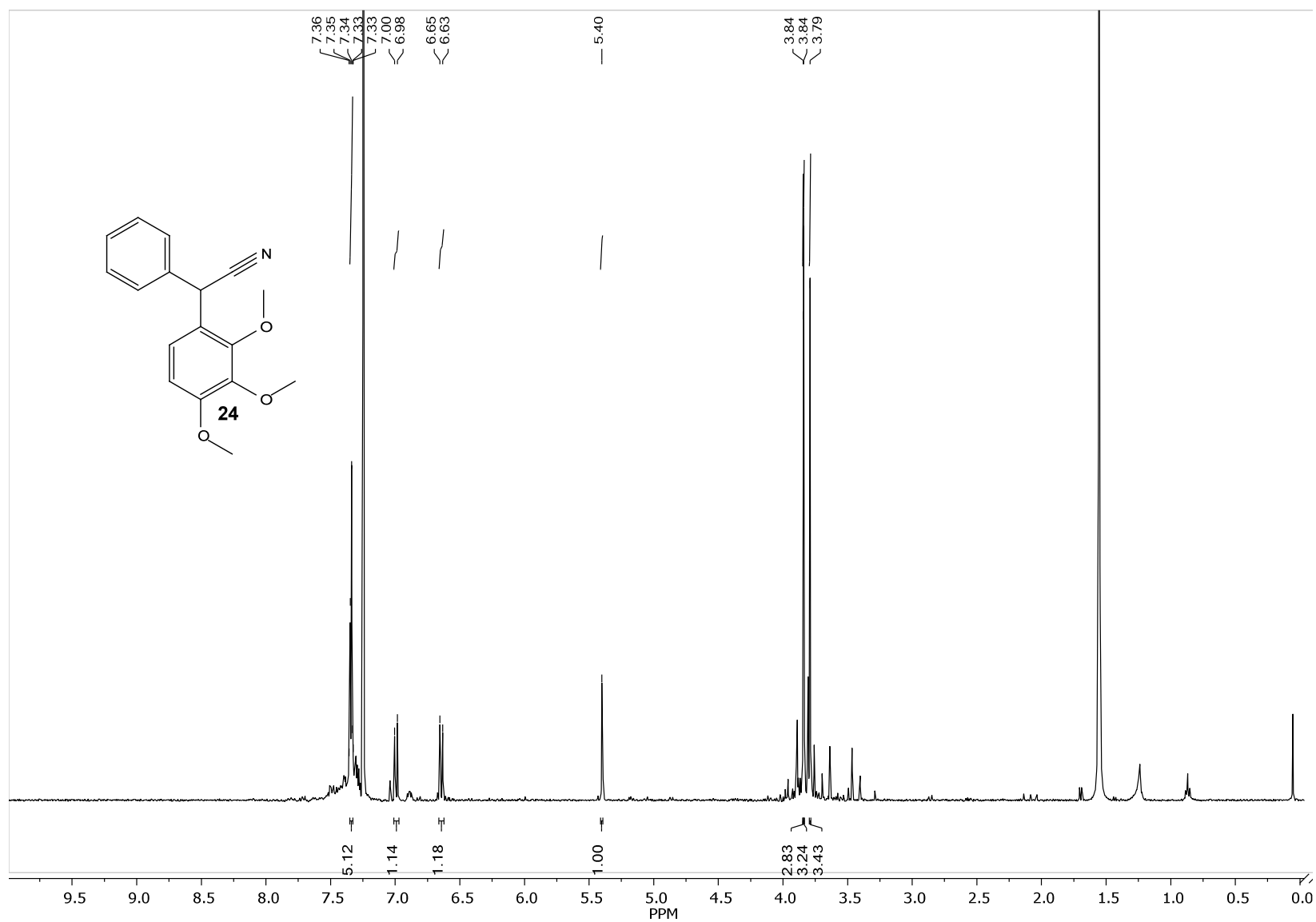
<sup>1</sup>H NMR for compounds **22/23**



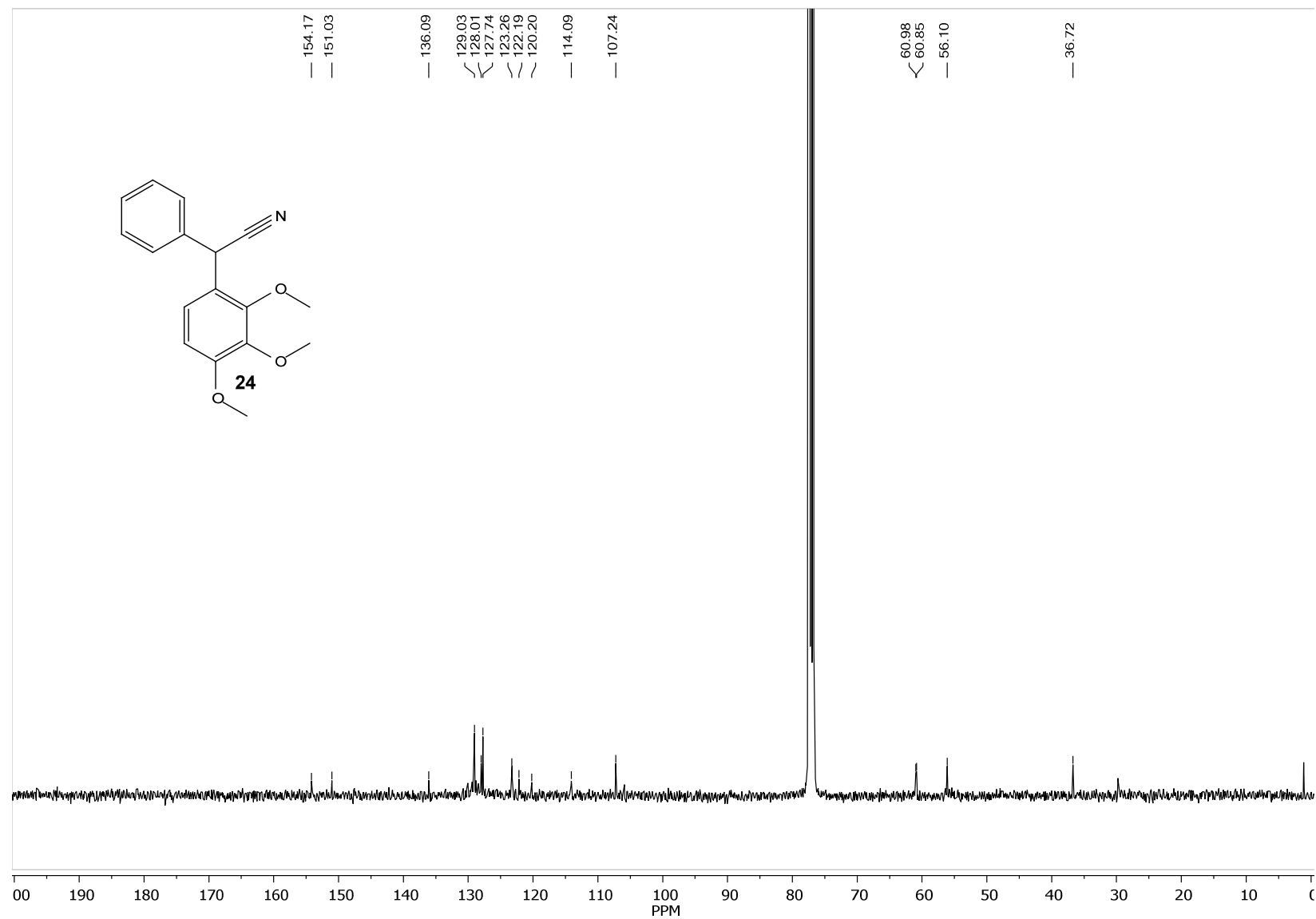
<sup>13</sup>C NMR for compounds **22/23**



<sup>1</sup>H NMR for compound **24**

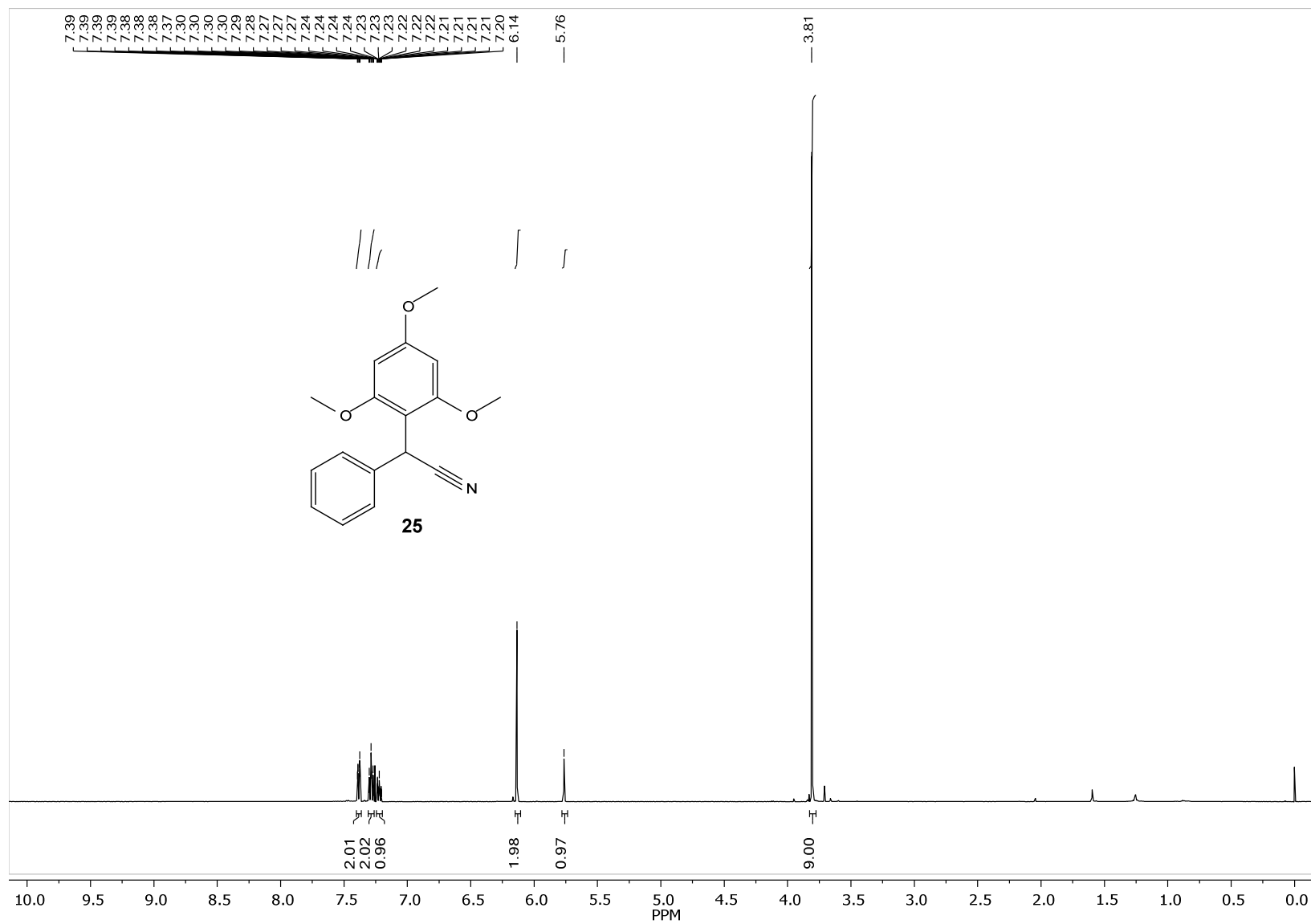


<sup>13</sup>C NMR for compound **24**

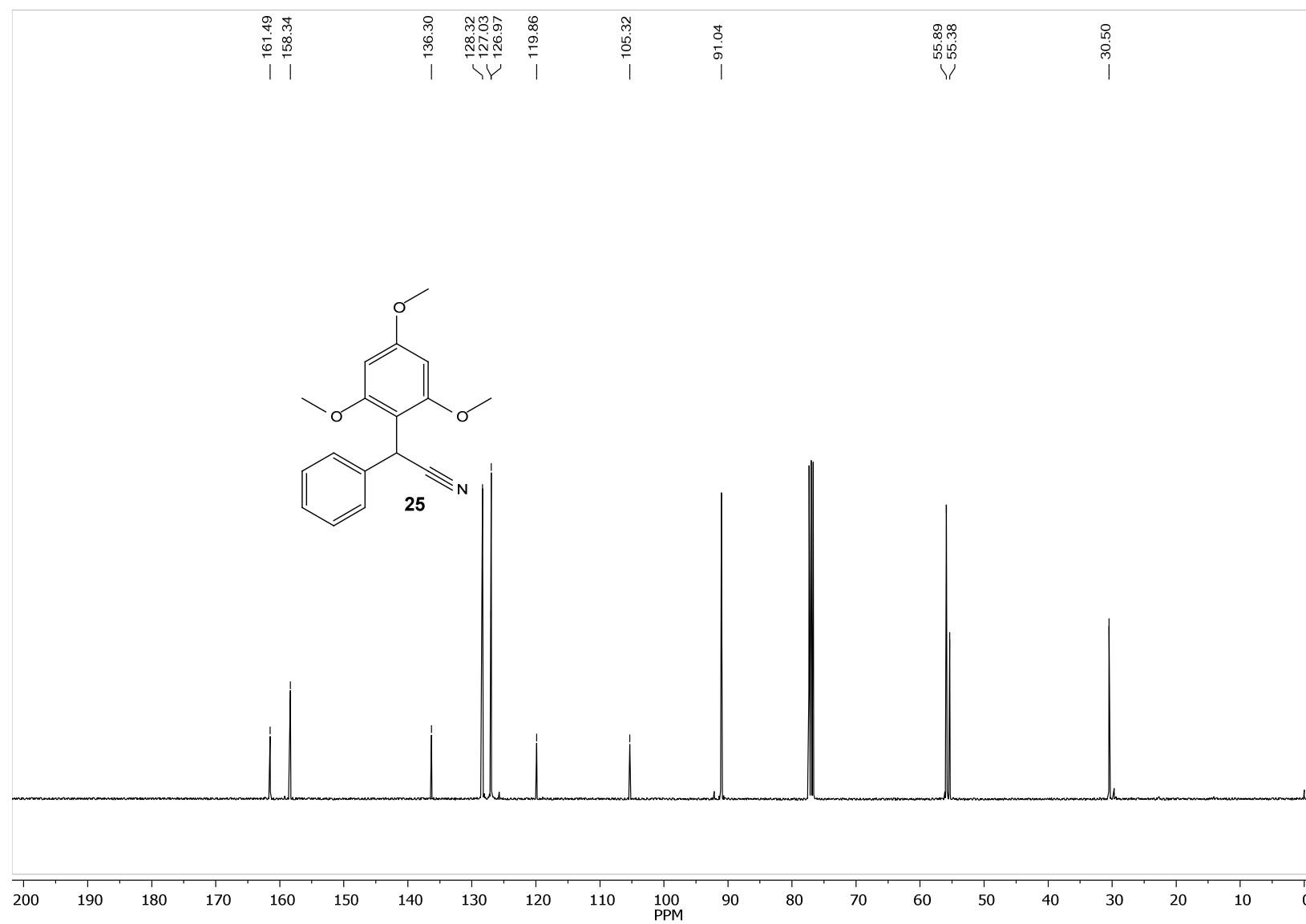




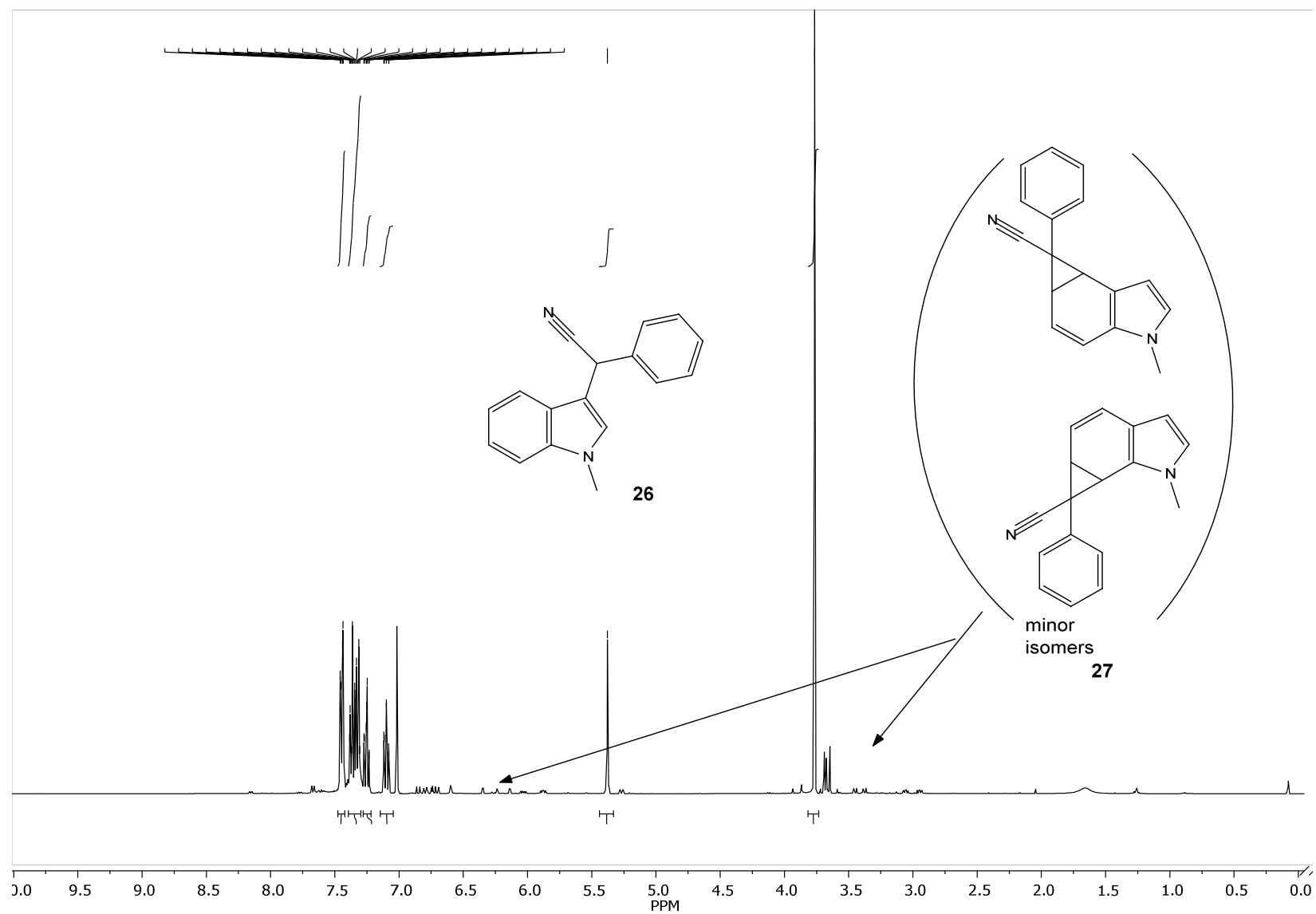
<sup>1</sup>H NMR for compound **25**



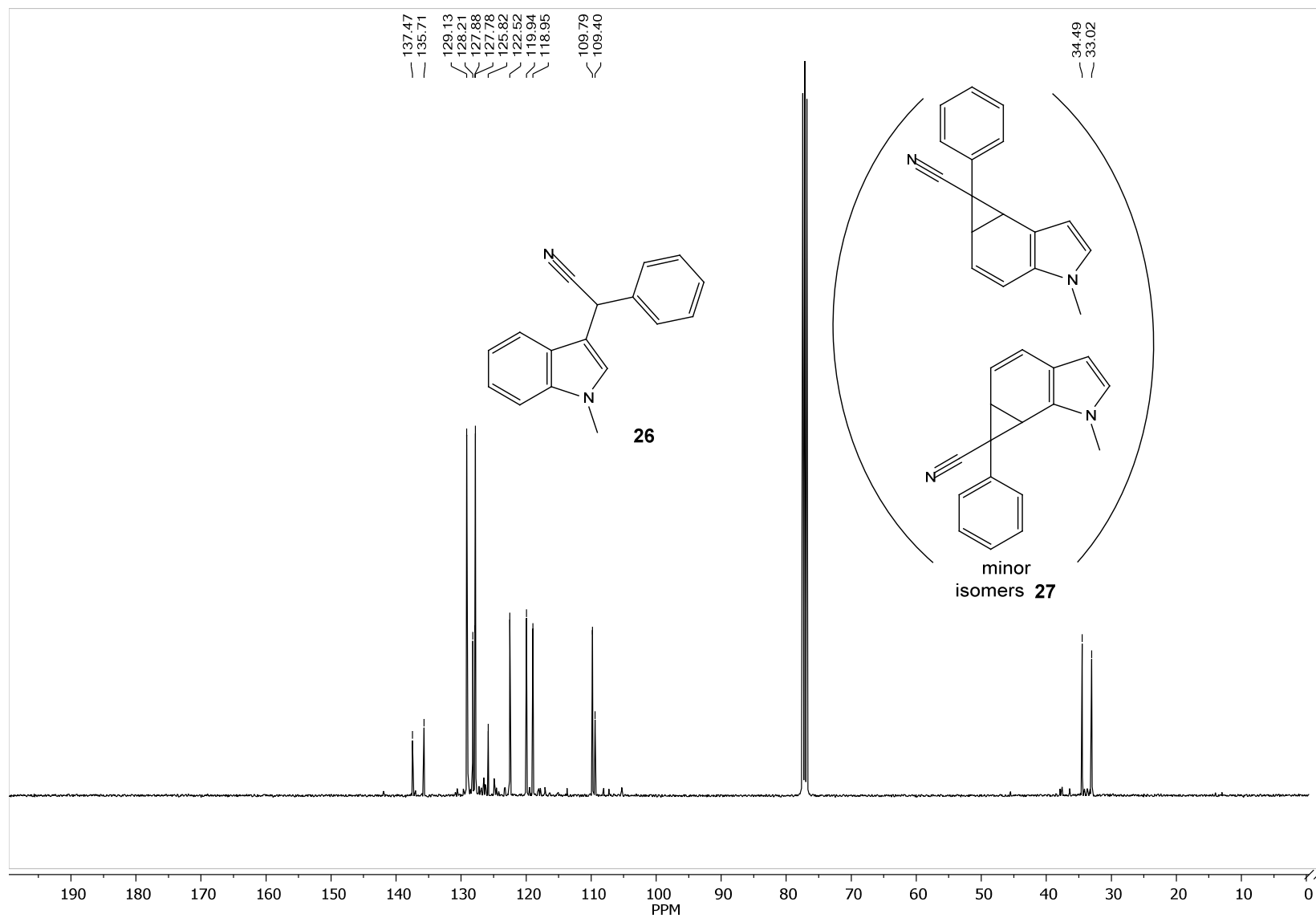
<sup>13</sup>C NMR for compound **25**



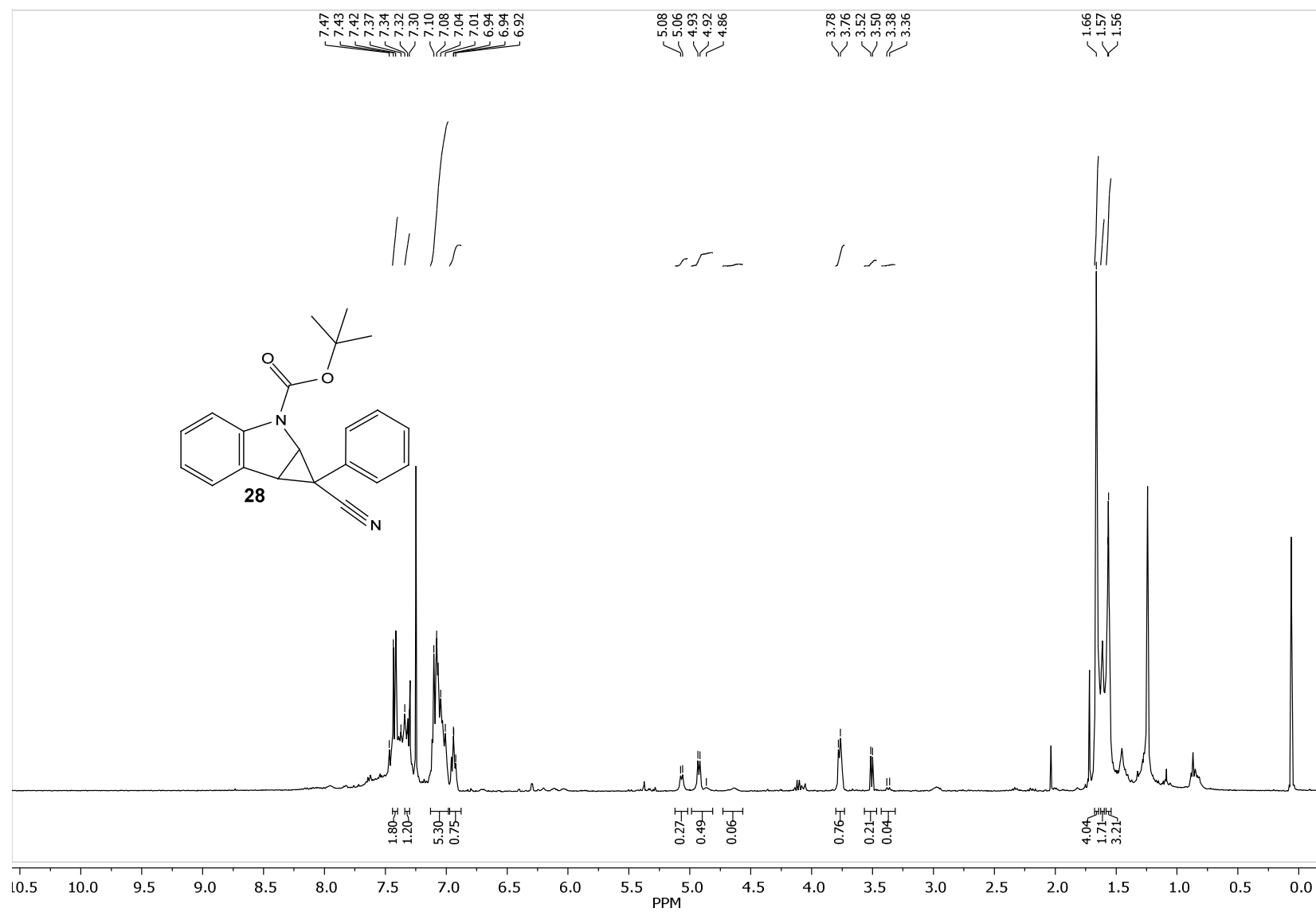
<sup>1</sup>H NMR for compounds **26/27**



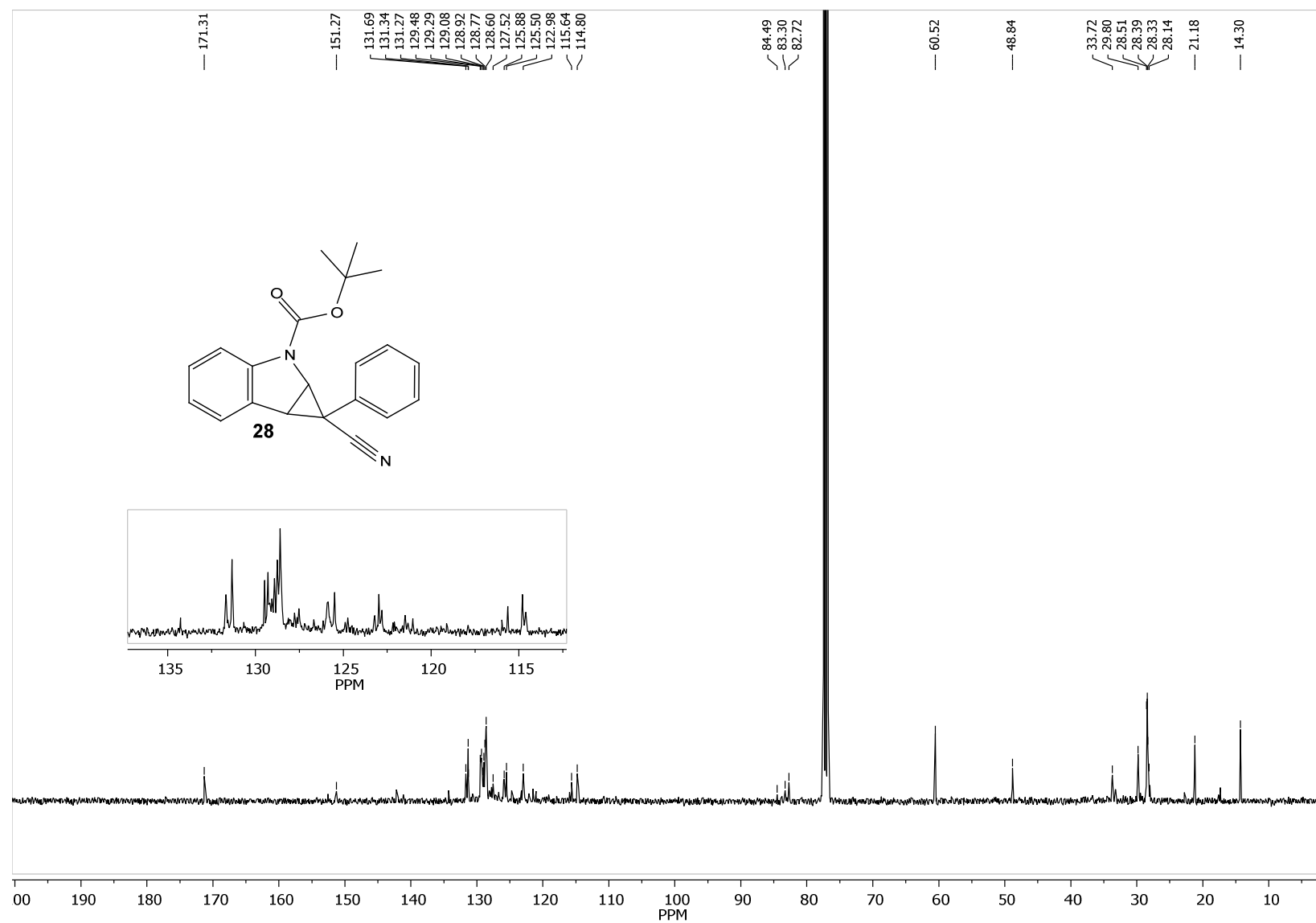
<sup>13</sup>C NMR for compounds **26/27**



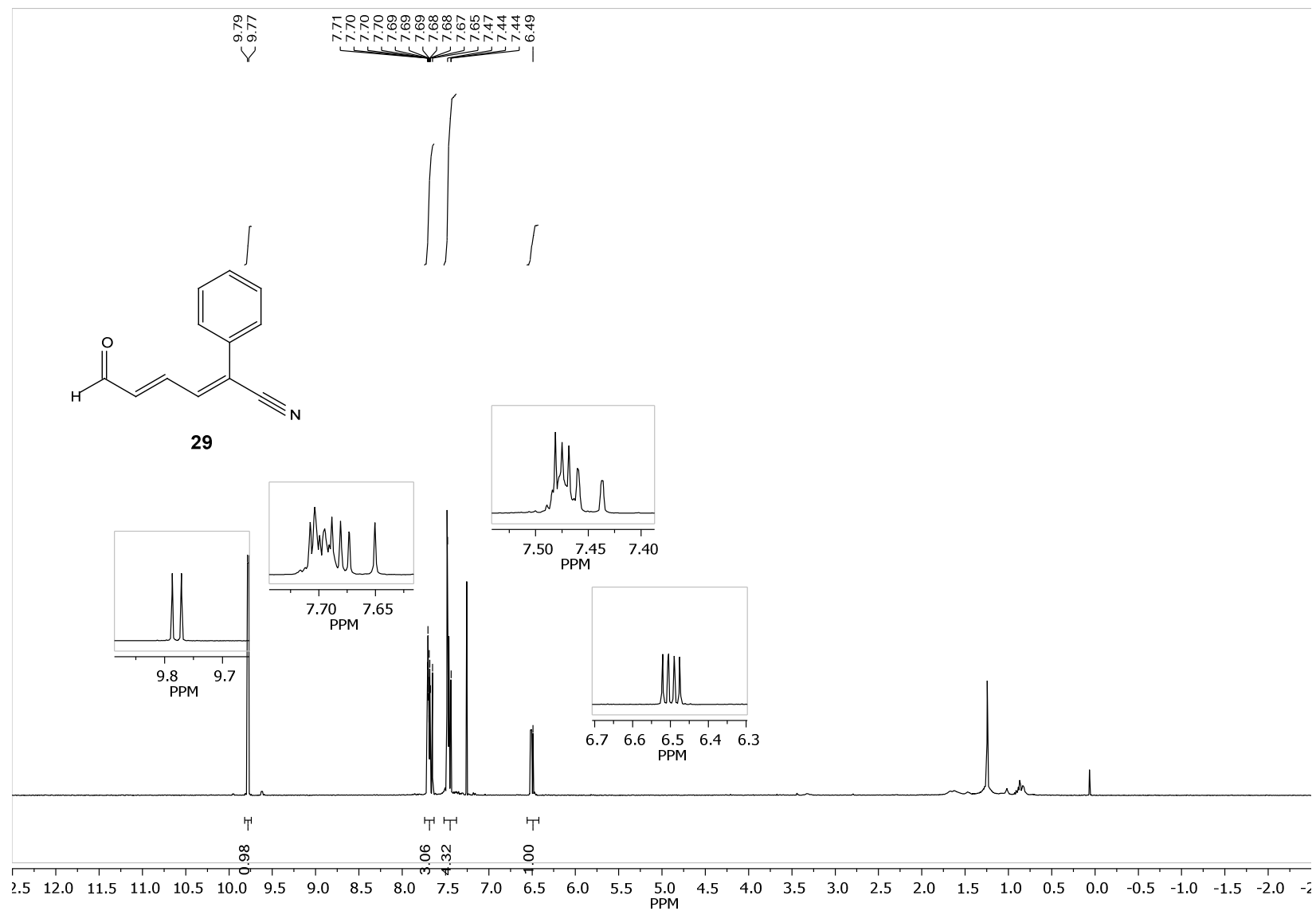
<sup>1</sup>H NMR for compounds **28** (mixture of diastereomers and rotamers)



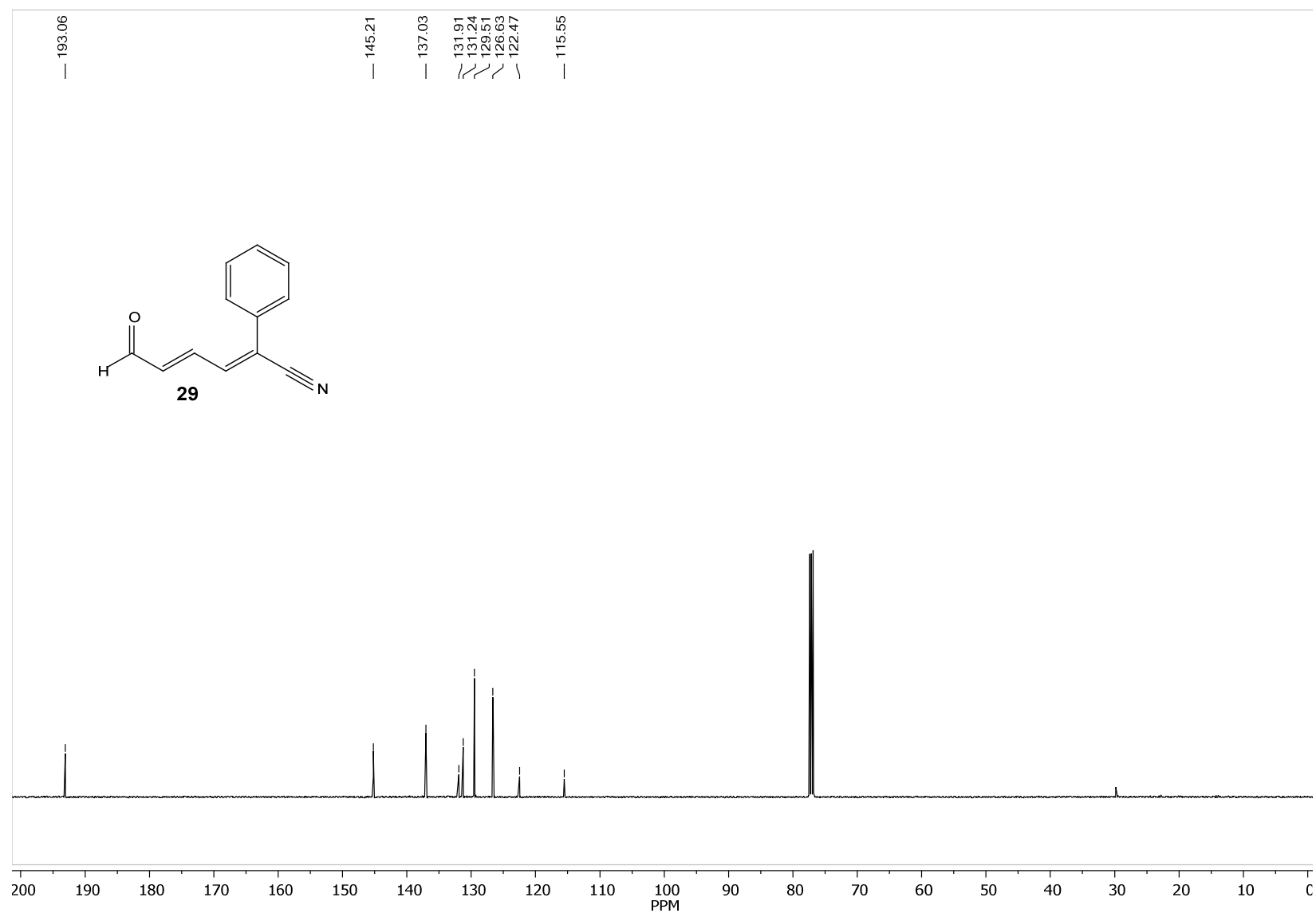
$^{13}\text{C}$  NMR for compounds **28** (*mixture of diastereomers and rotamers*)



<sup>1</sup>H NMR for compounds **29**

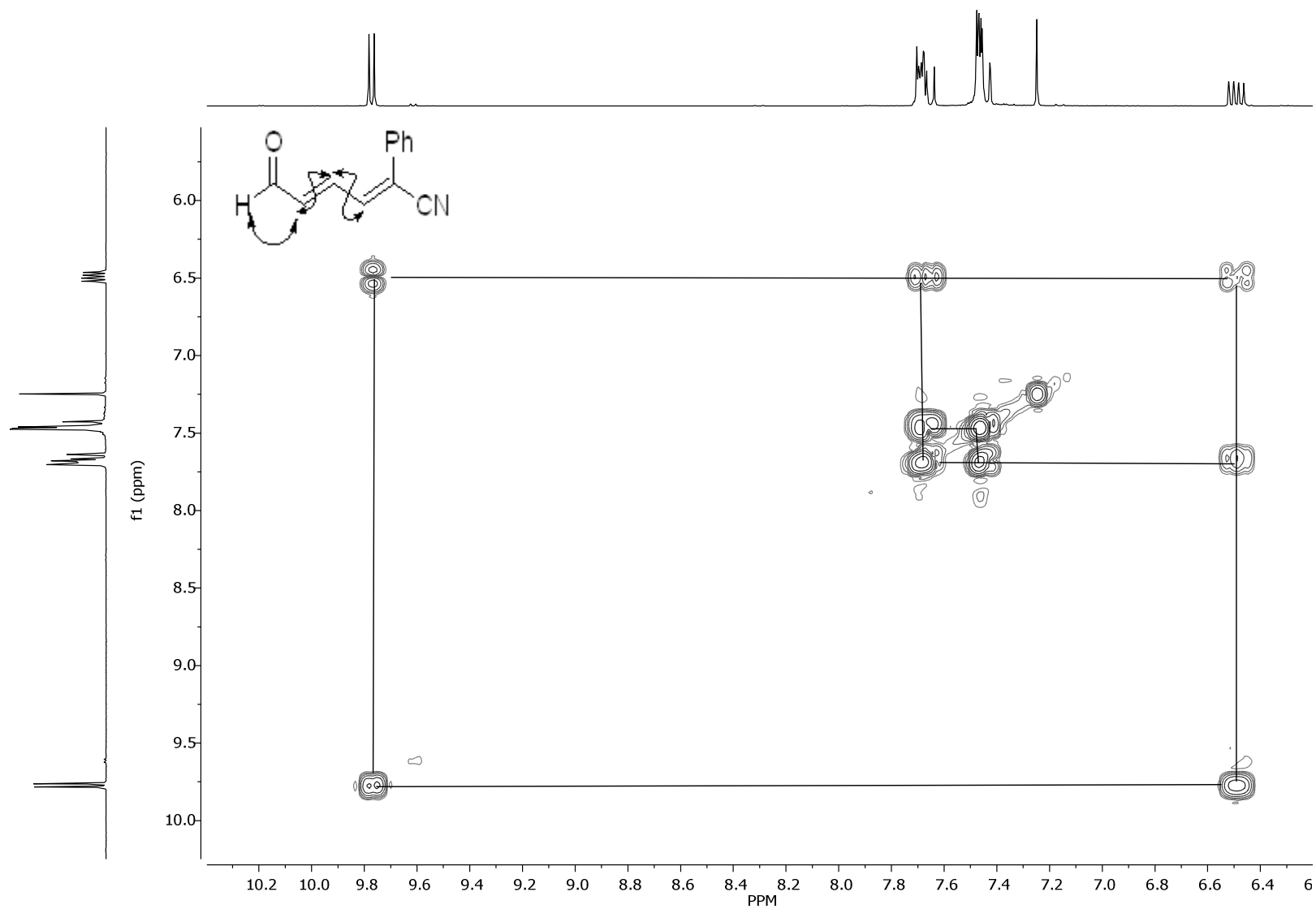


<sup>13</sup>C NMR for compounds **29**

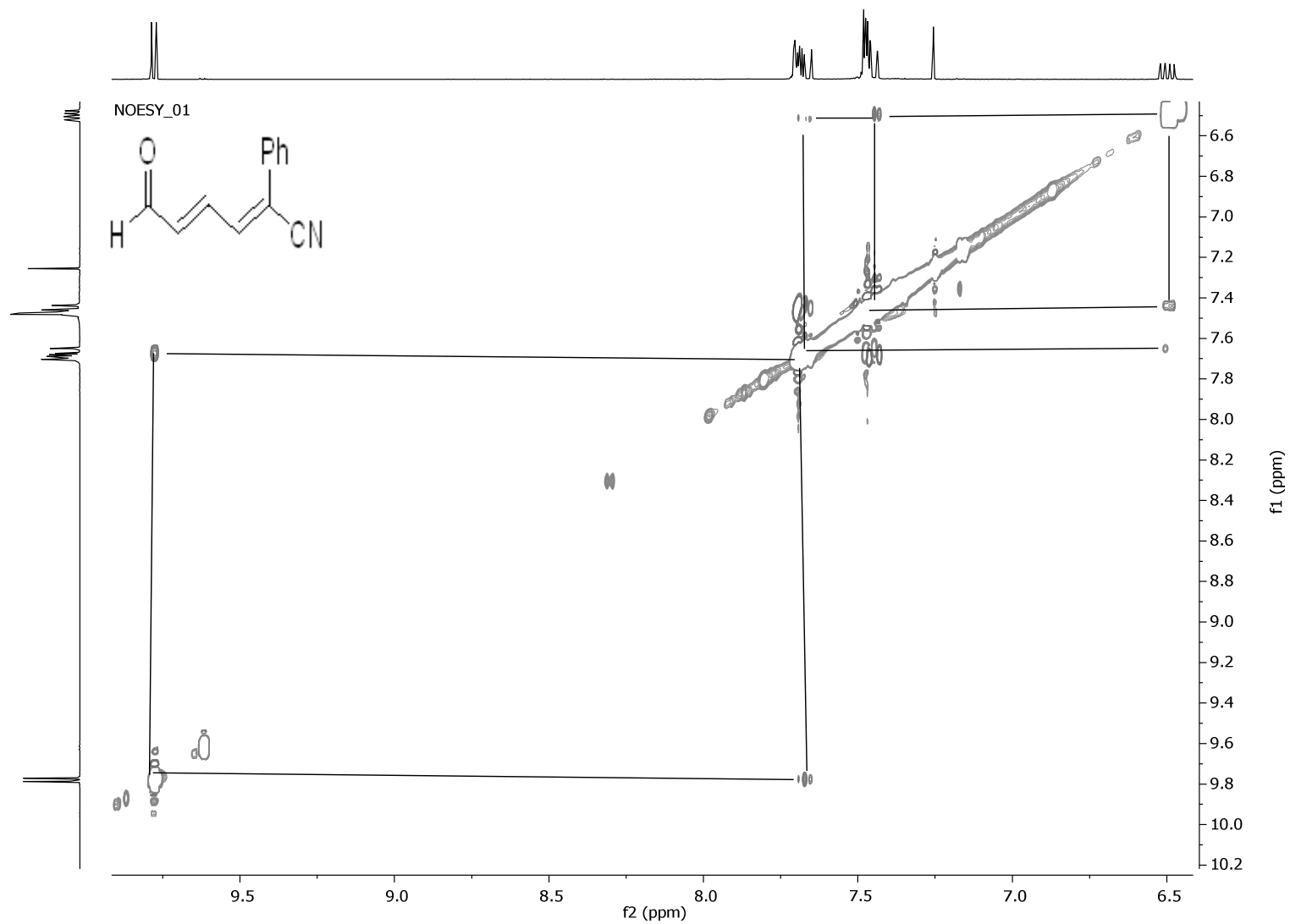




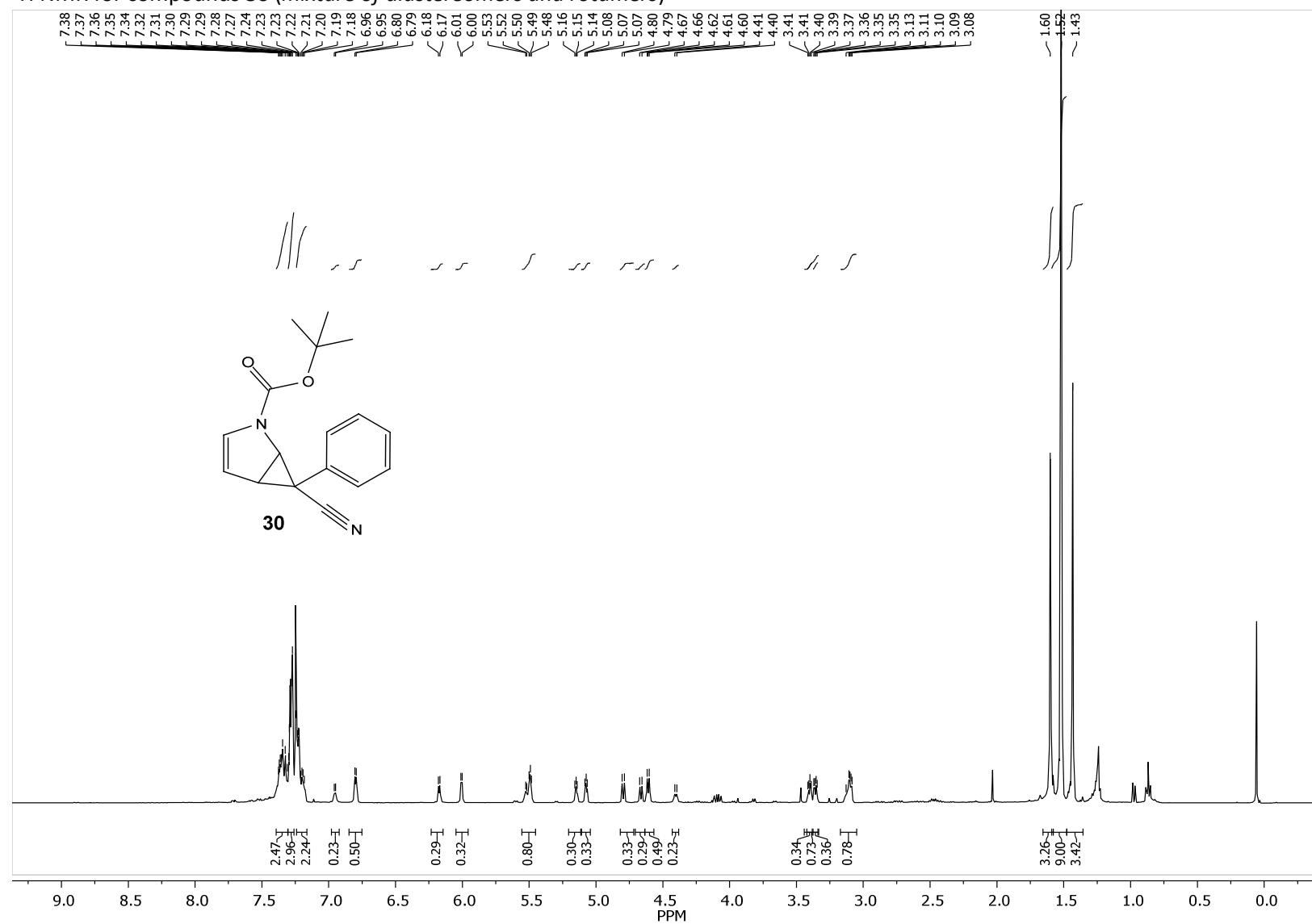
$^1\text{H}$ - $^1\text{H}$  COSY for compound **29**



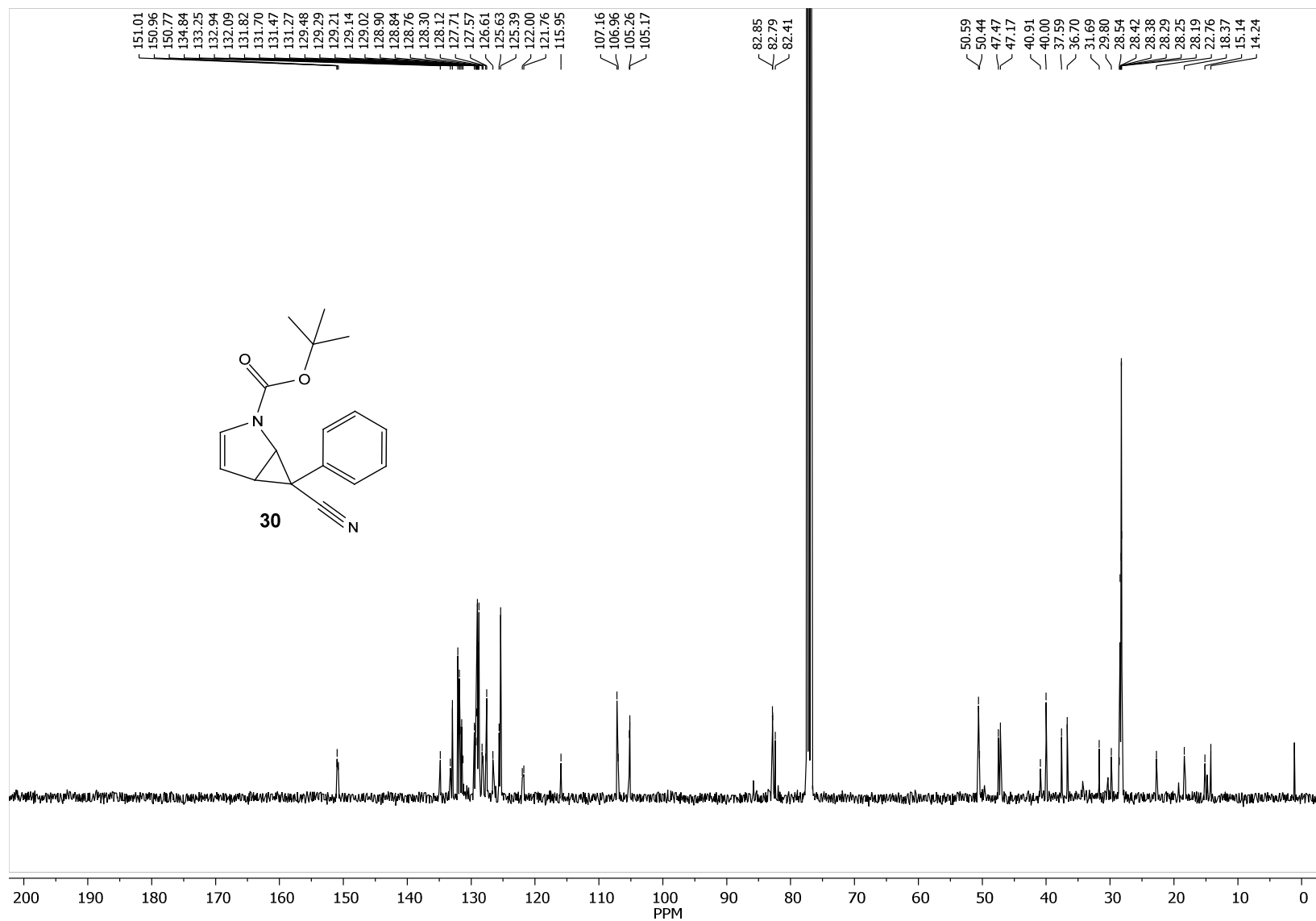
NOESY for compound **29**



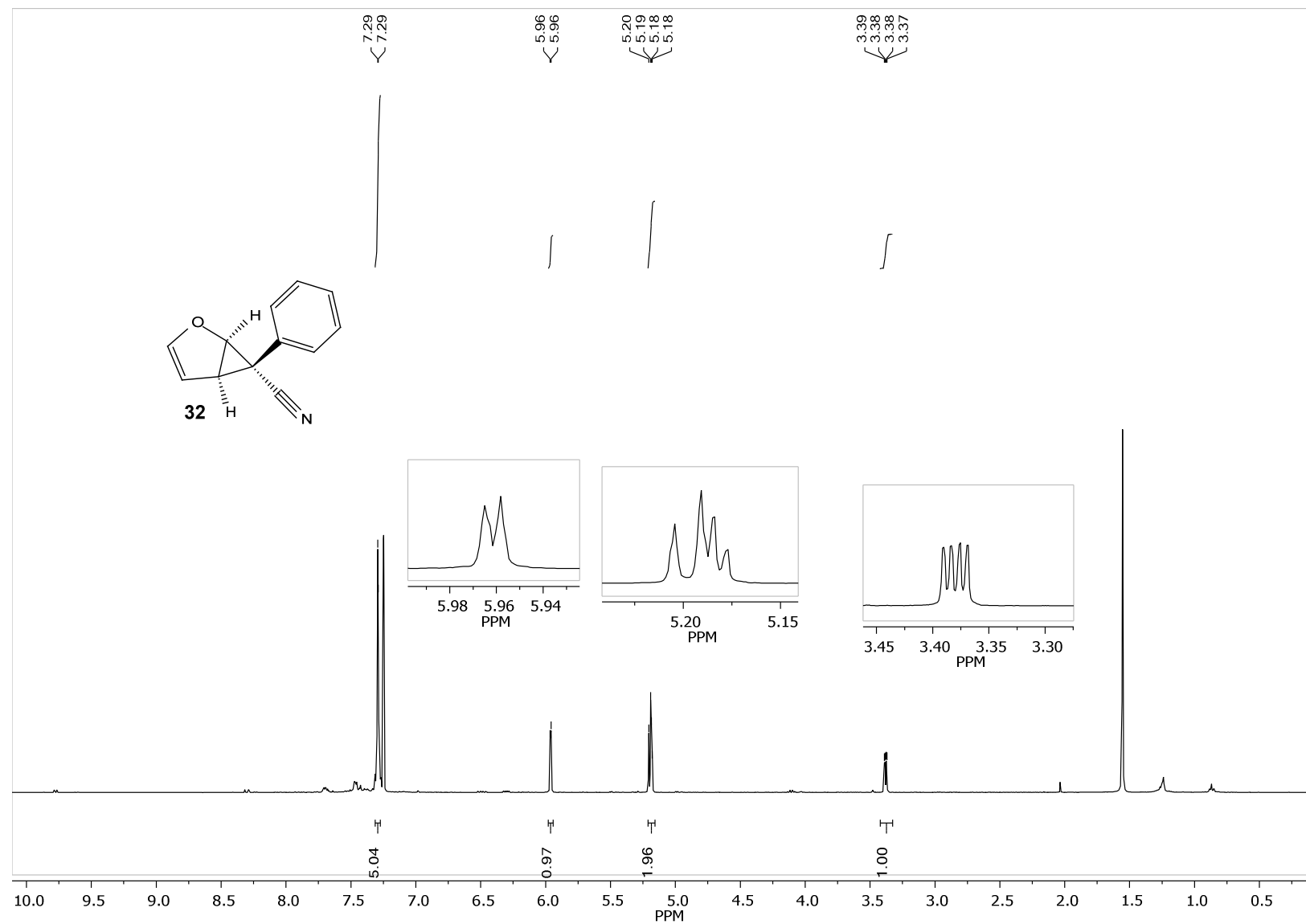
<sup>1</sup>H NMR for compounds **30** (mixture of diastereomers and rotamers)



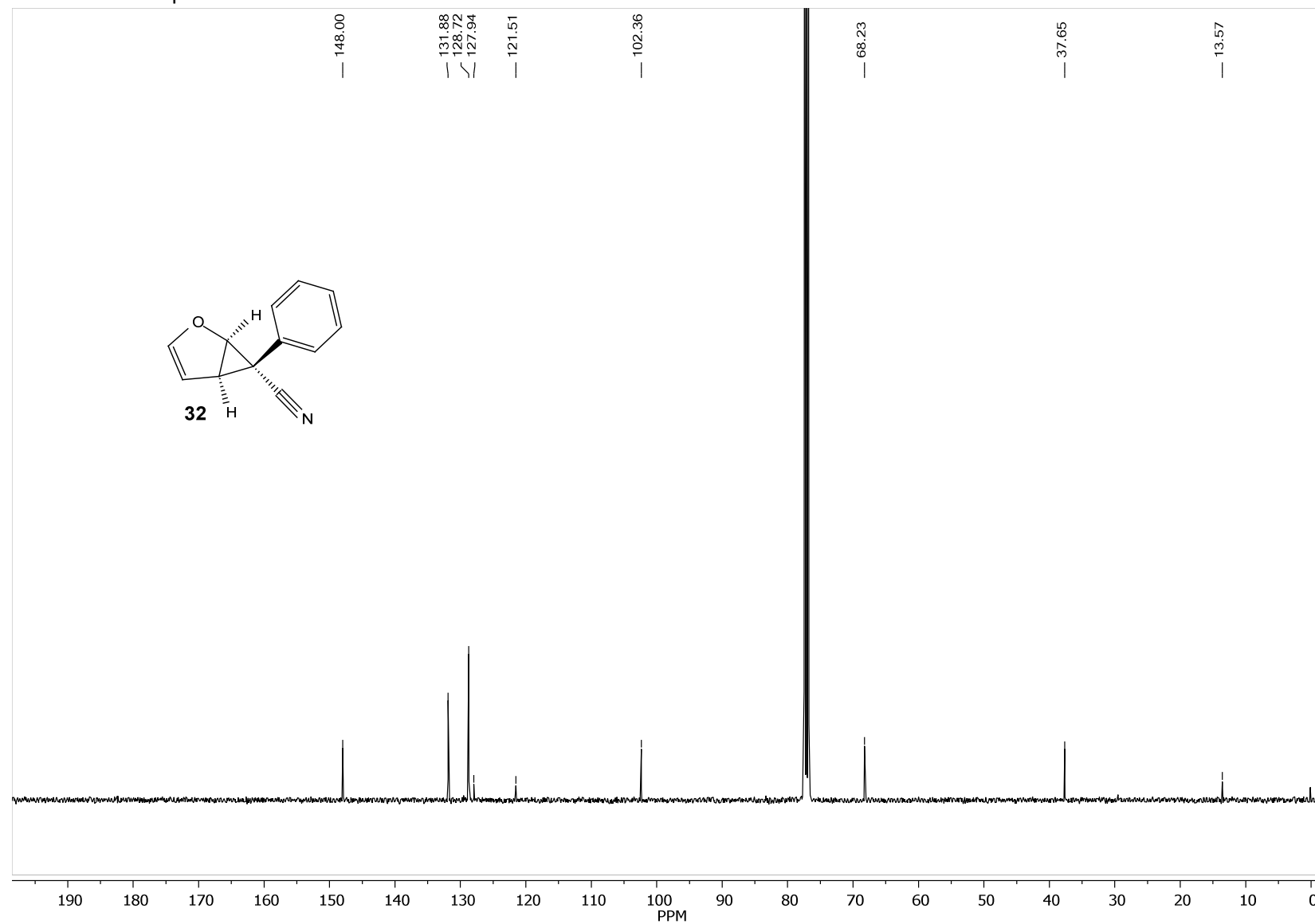
$^{13}\text{C}$  NMR for compounds **30** (*mixture of diastereomers and rotamers*)



<sup>1</sup>H NMR for compounds **32**



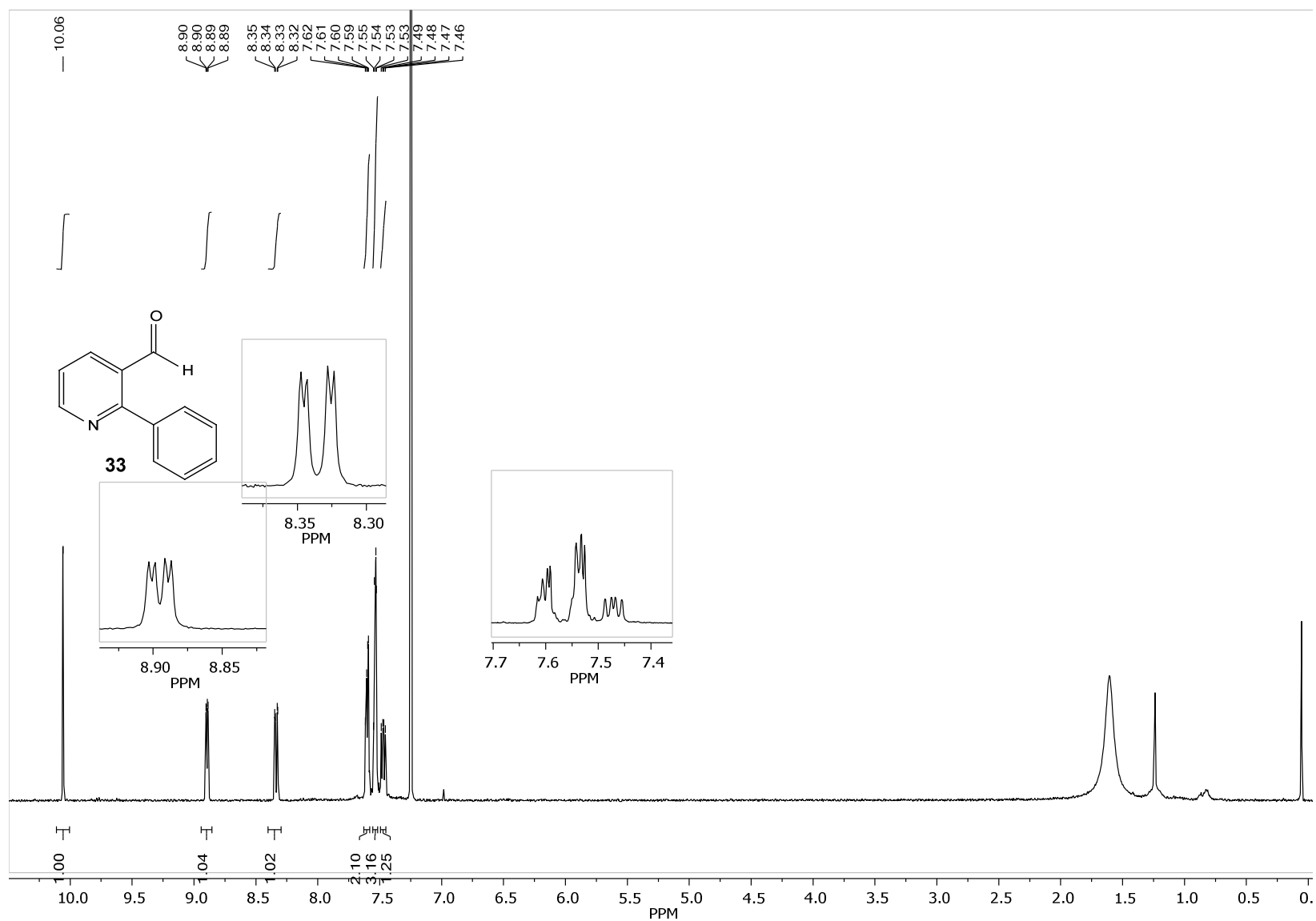
<sup>13</sup>C NMR for compounds **32**



$^1\text{H}$ - $^1\text{H}$  COSY for compounds **32**

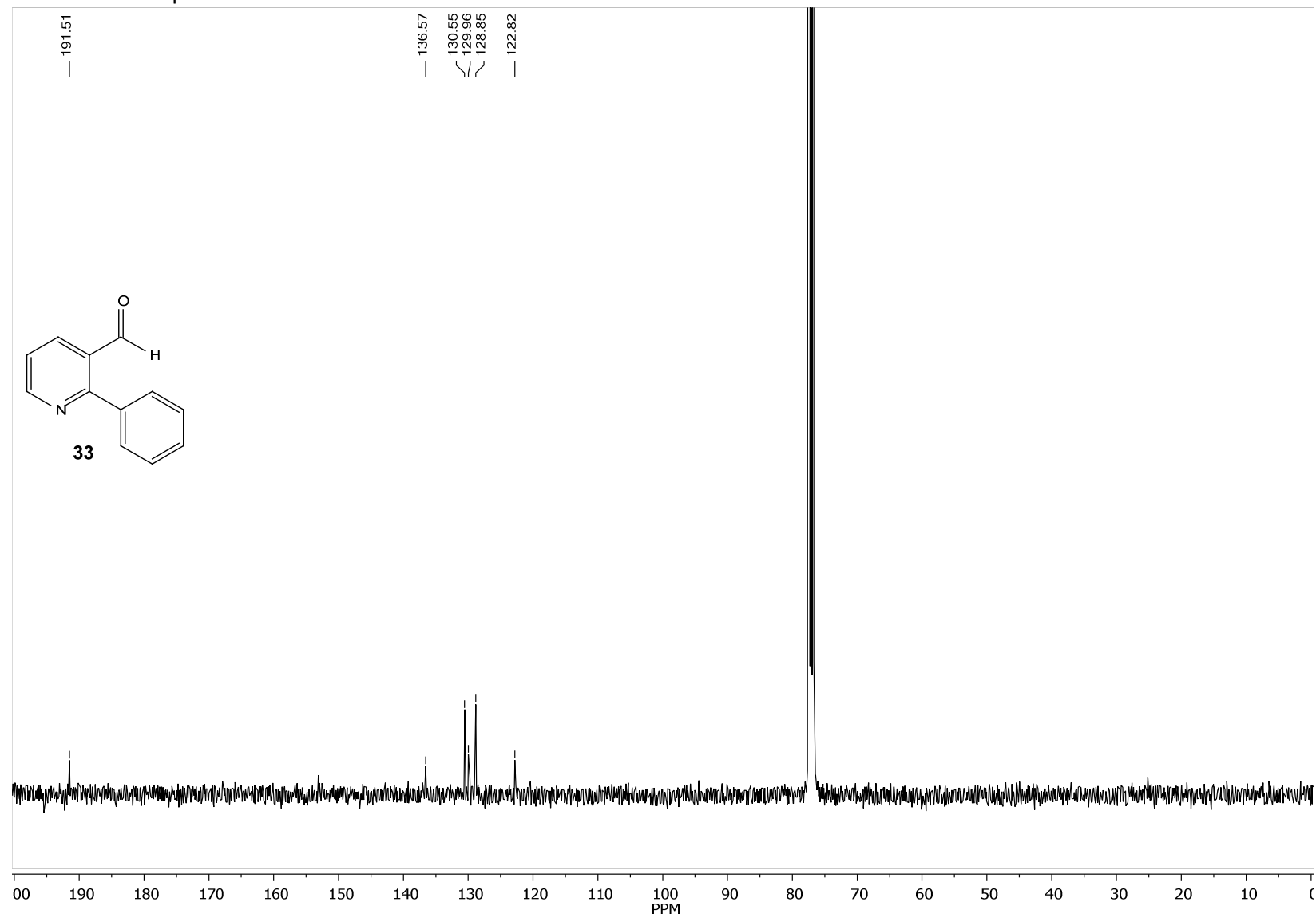


<sup>1</sup>H NMR for compounds **33**

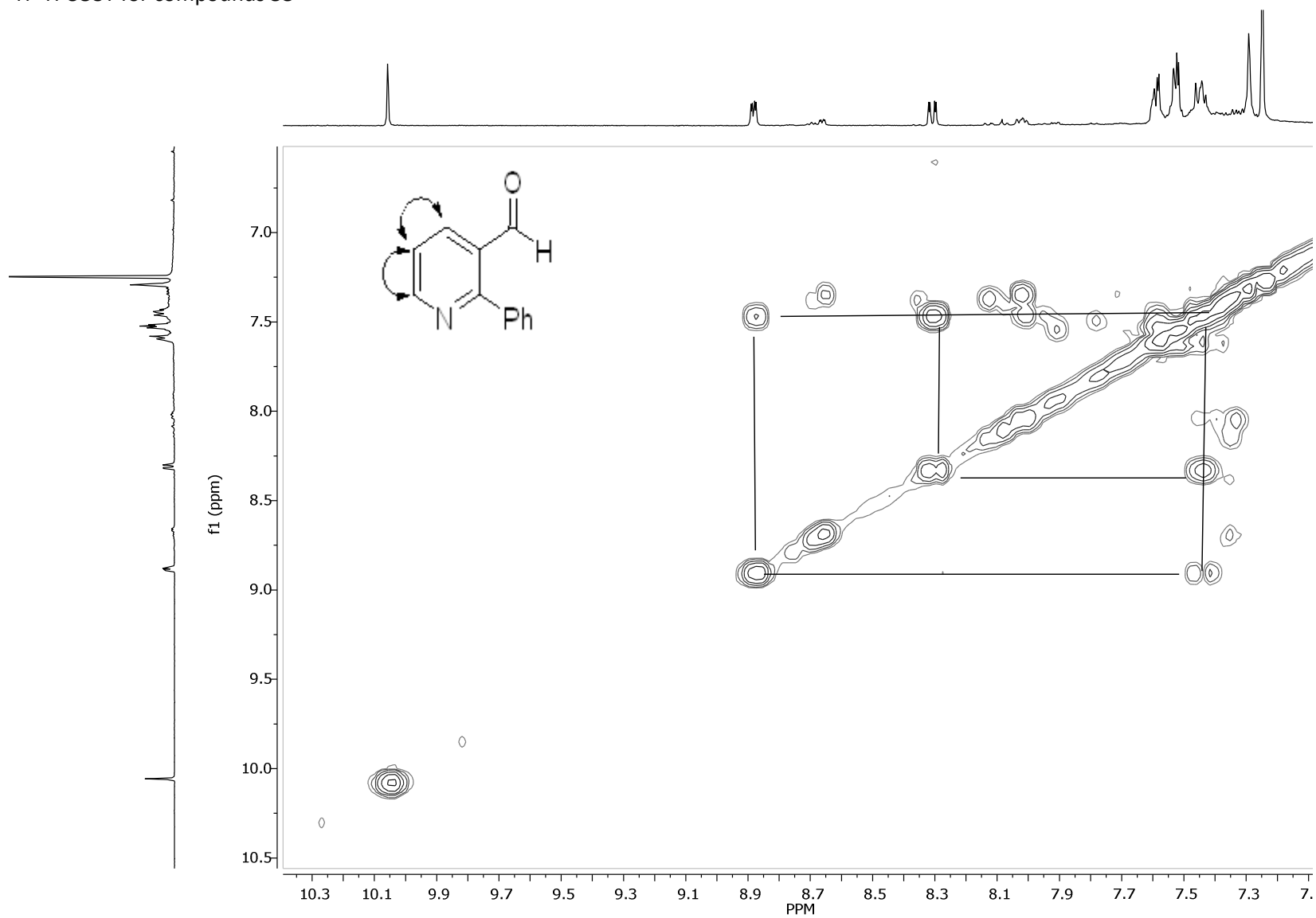




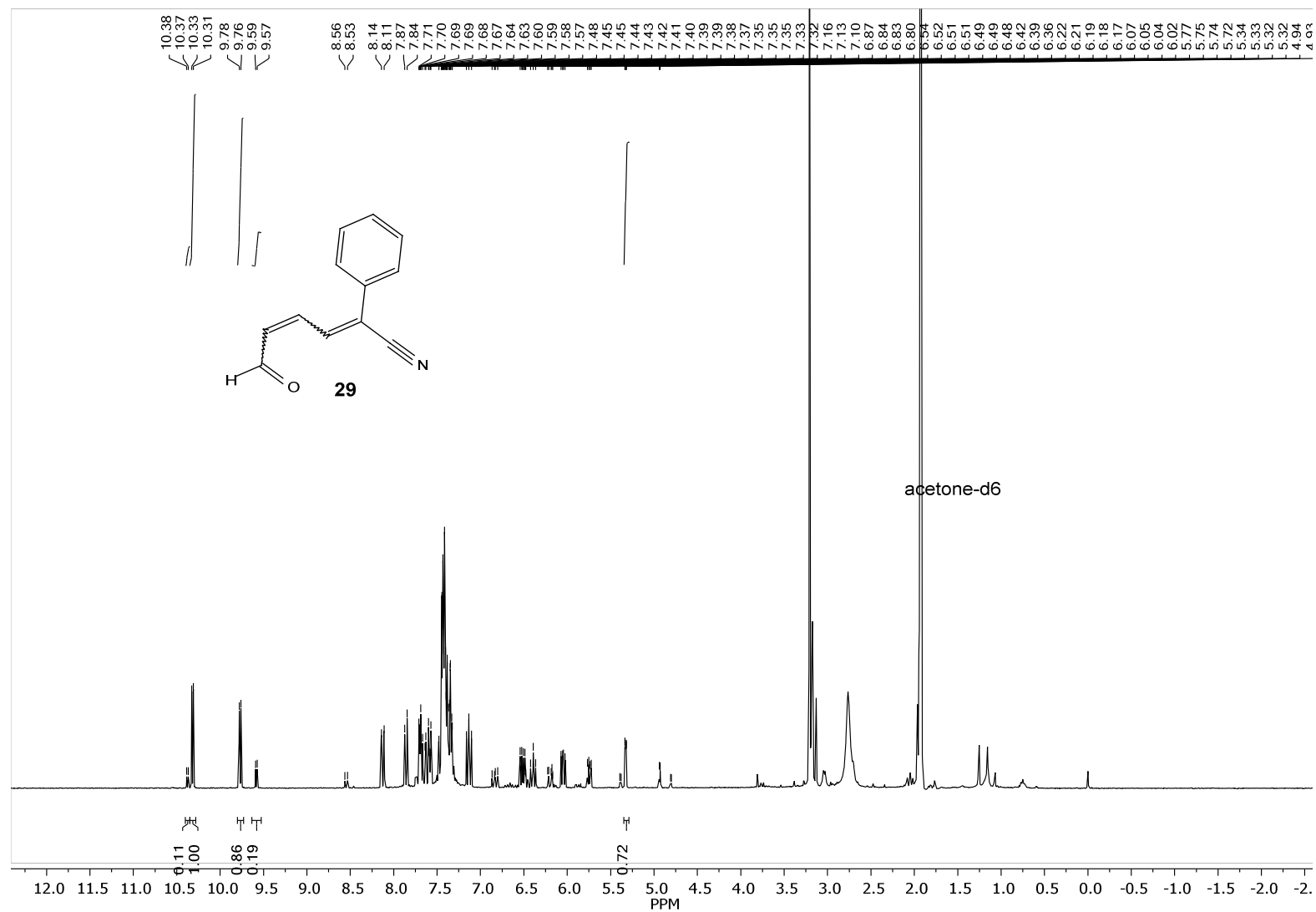
<sup>13</sup>C NMR for compounds **33**



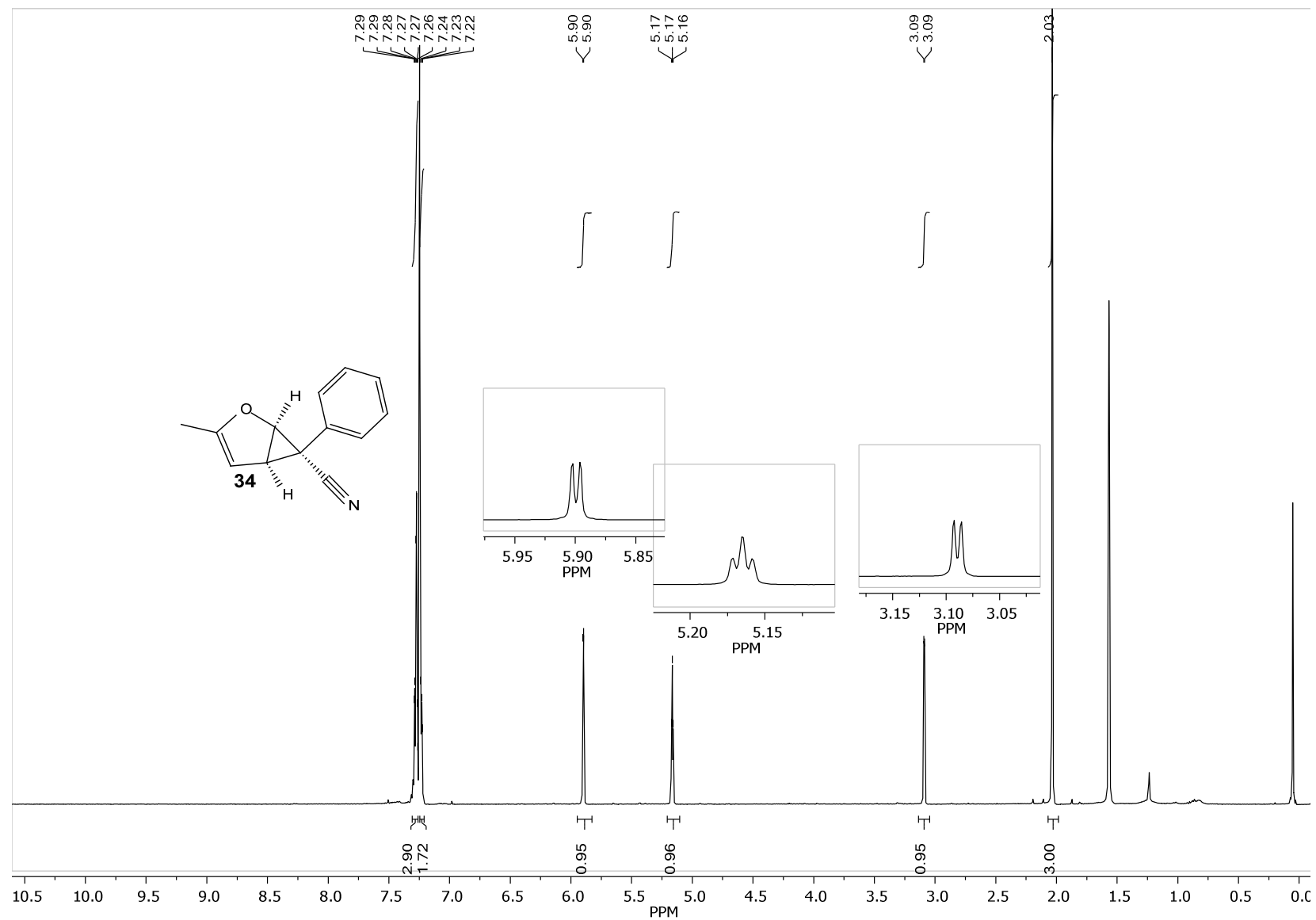
$^1\text{H}$ - $^1\text{H}$  COSY for compounds **33**



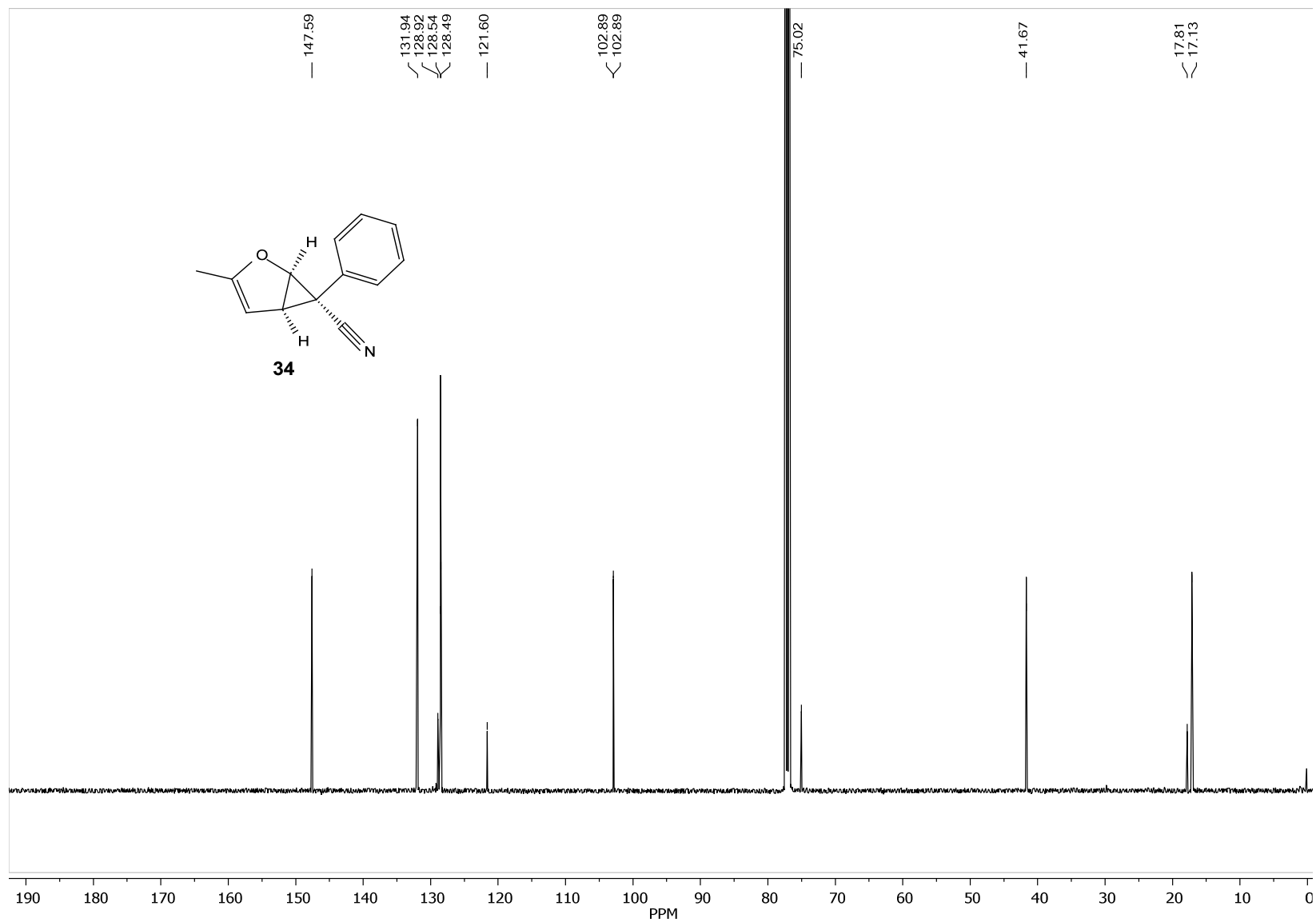
<sup>1</sup>H NMR for all isomers of **29** (isolated from the cyanocarbene reaction with furan)



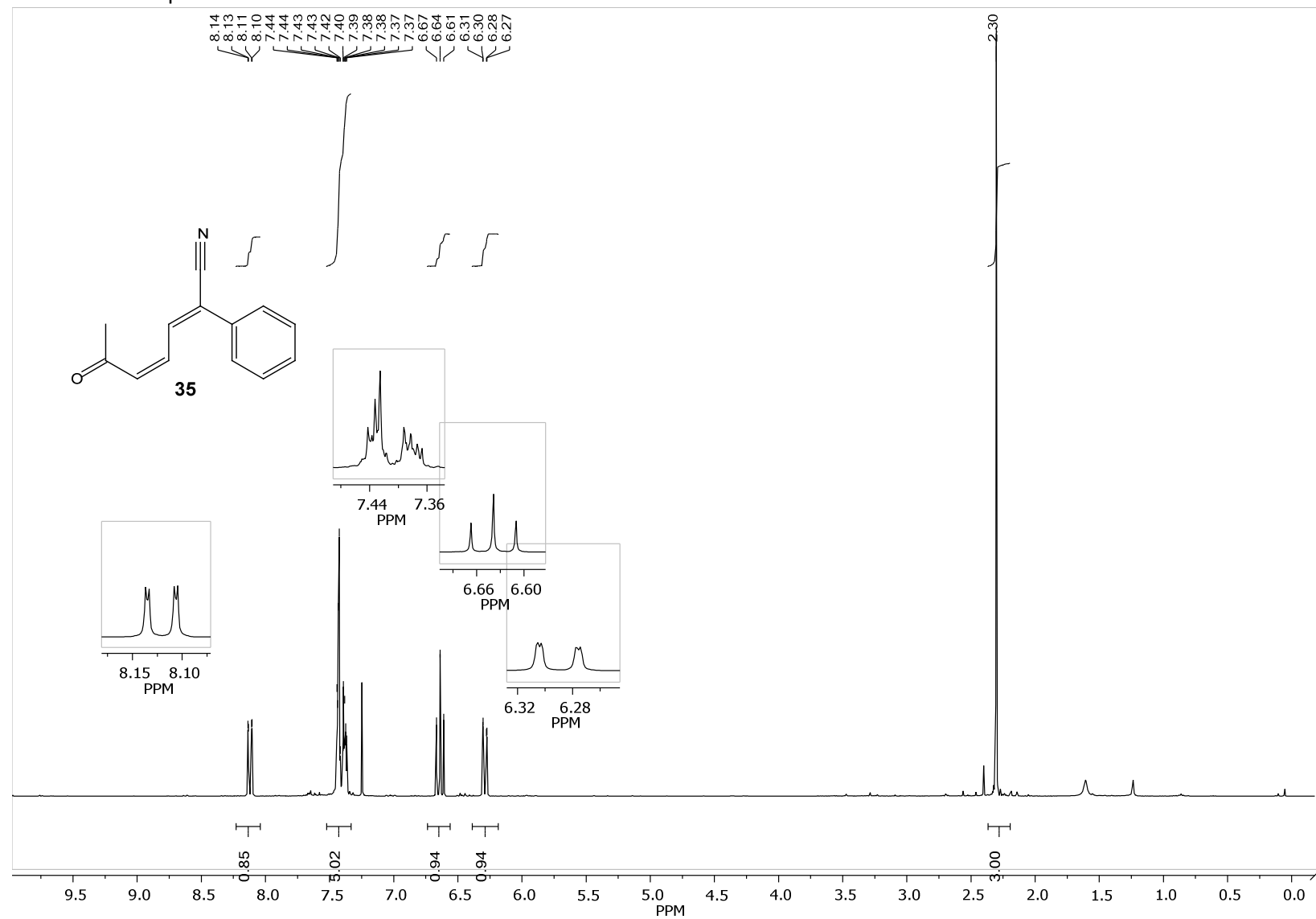
<sup>1</sup>H NMR for compounds **34**



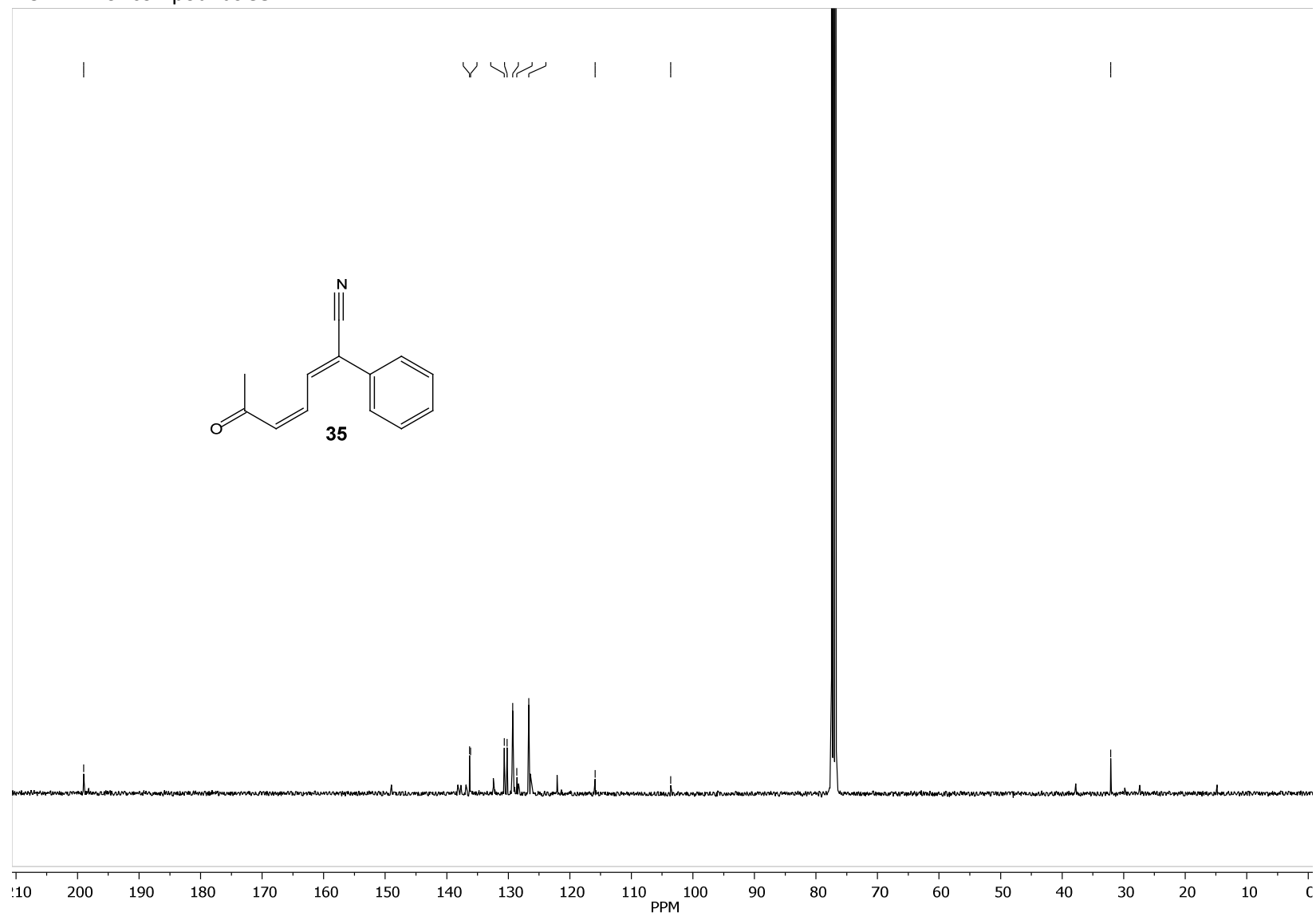
<sup>13</sup>C NMR for compounds **34**



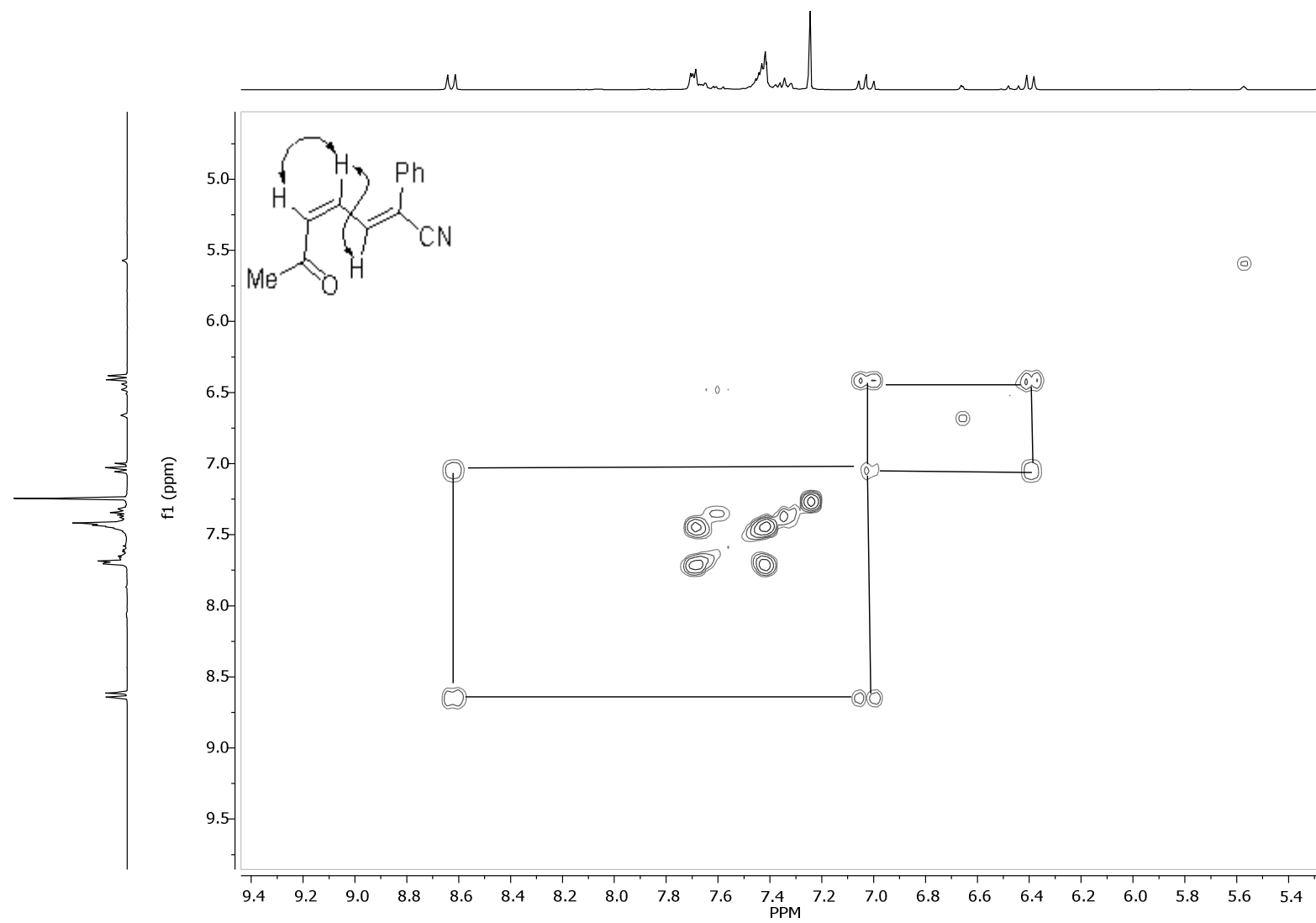
<sup>1</sup>H NMR for compounds **35**



<sup>13</sup>C NMR for compounds **35**

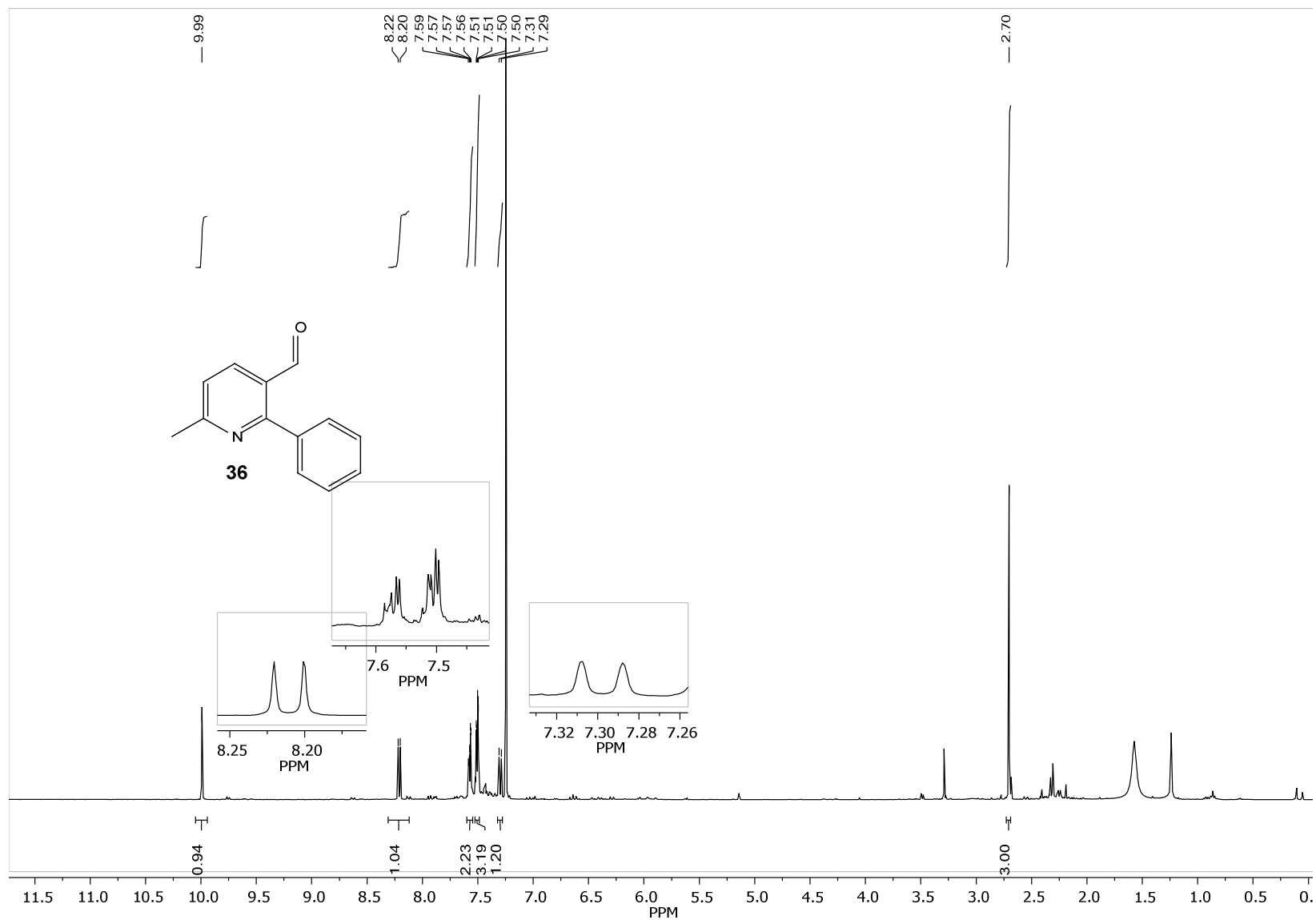


$^1\text{H}$ - $^1\text{H}$  COSY for compounds **35**

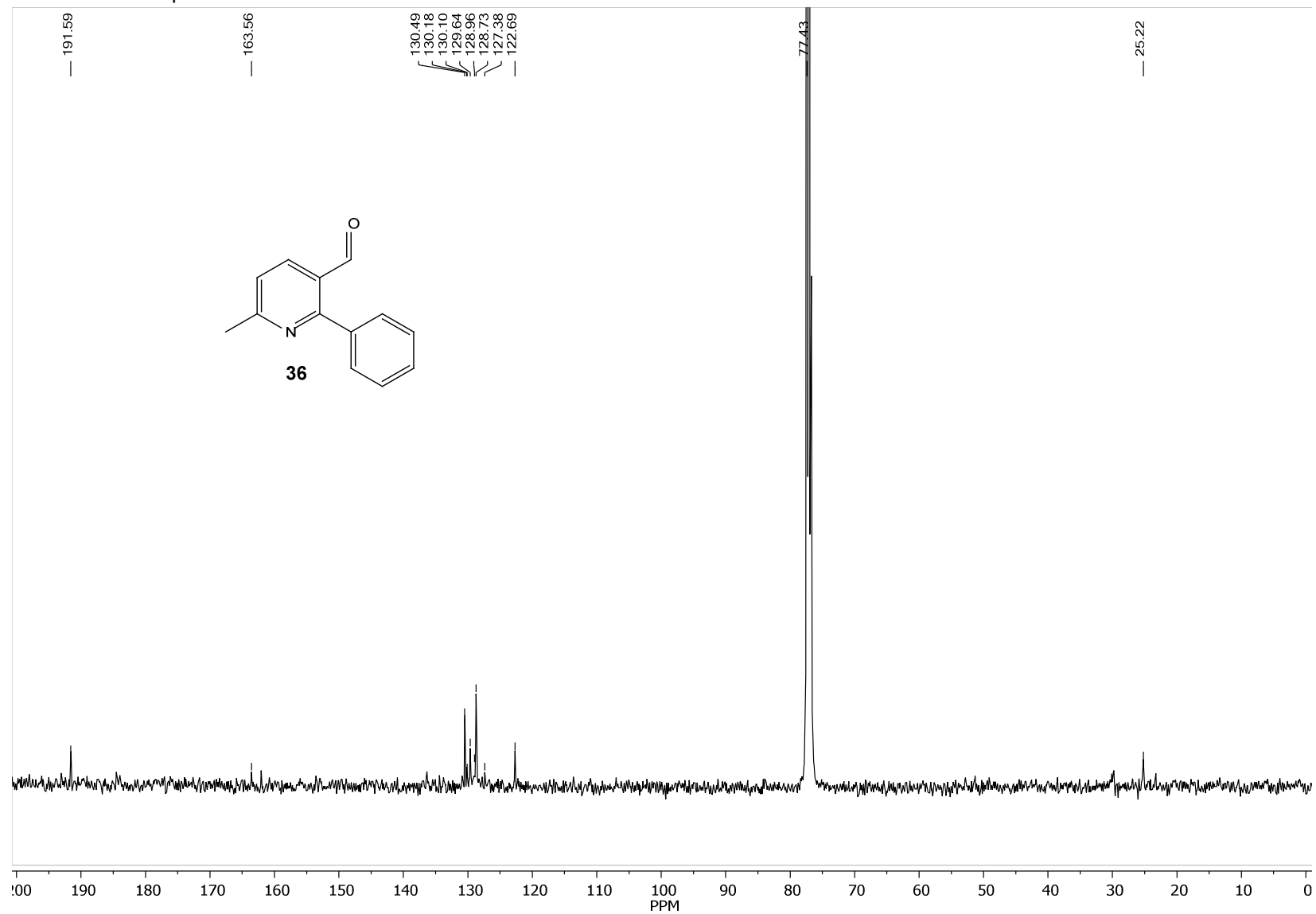




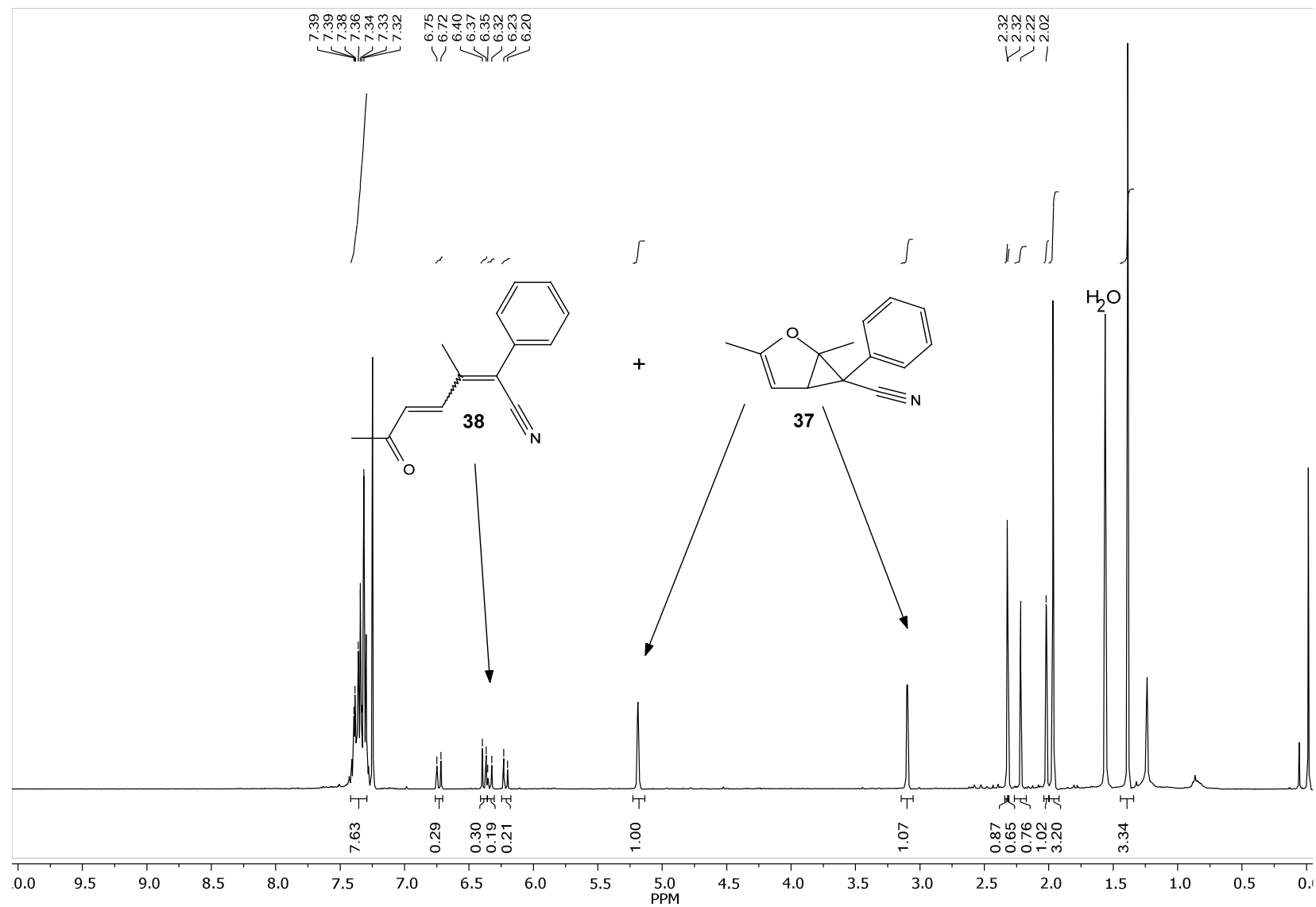
<sup>1</sup>H NMR for compounds **36**



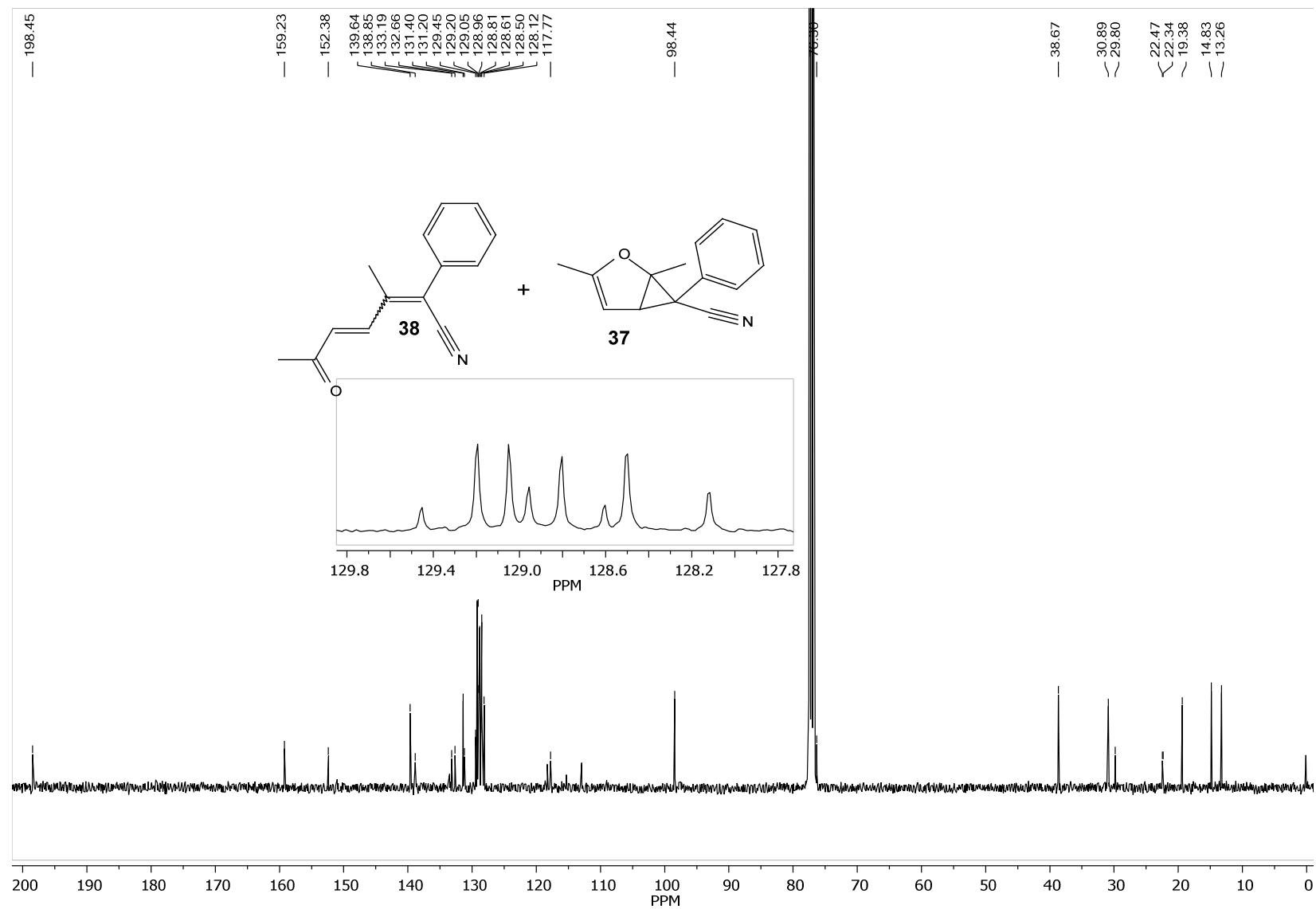
<sup>13</sup>C NMR for compounds **36**



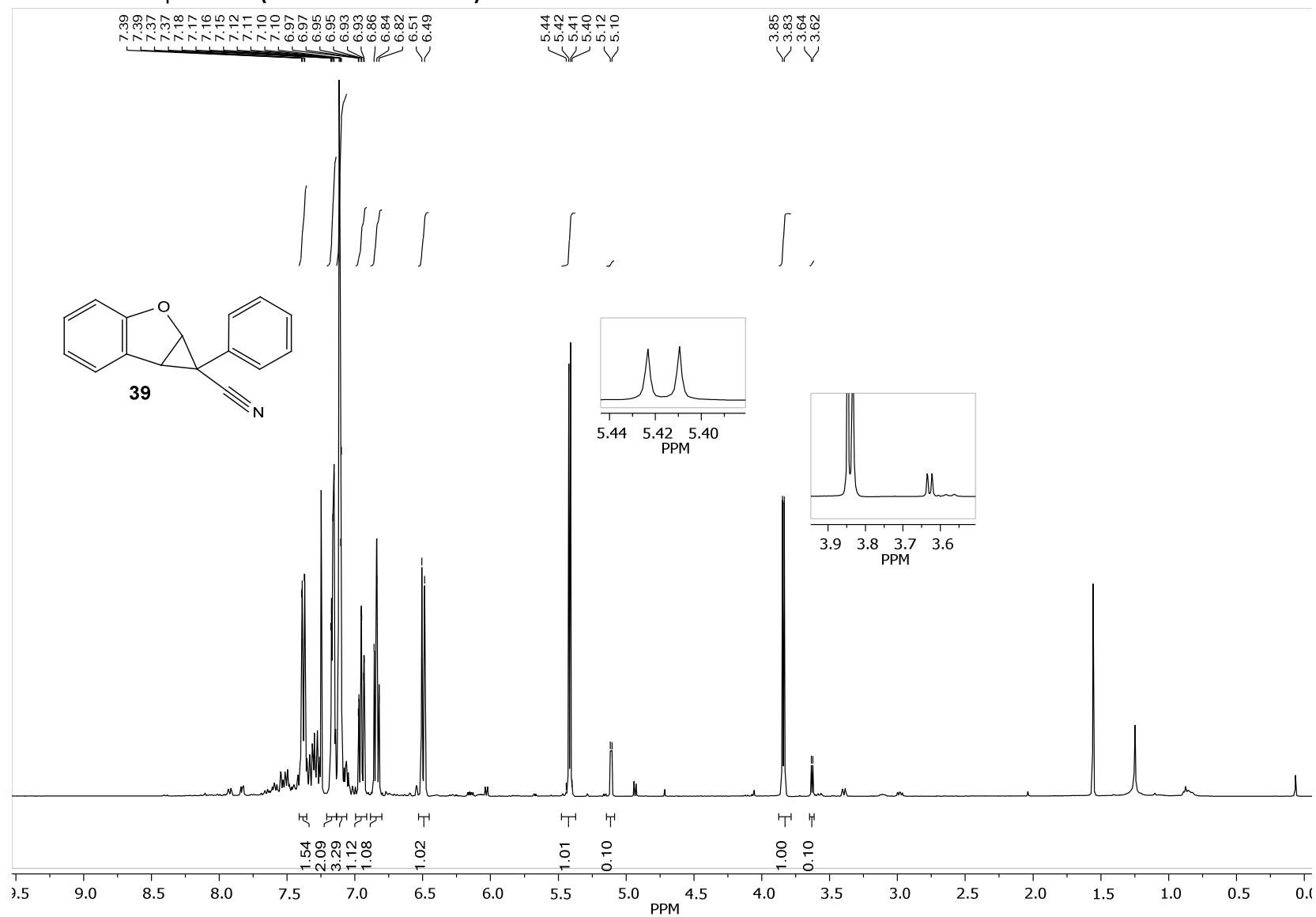
<sup>1</sup>H NMR for compounds **37/38**



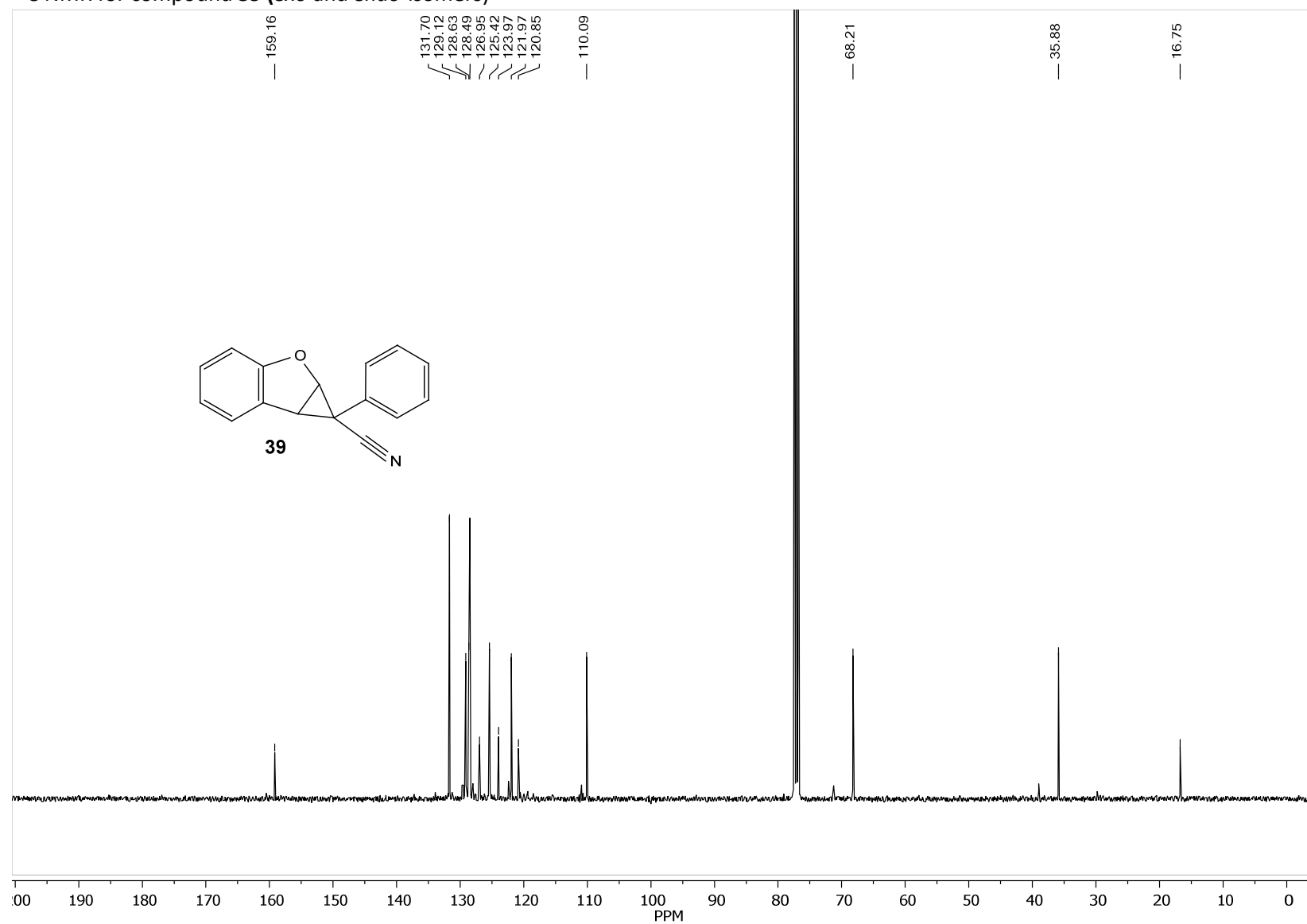
<sup>13</sup>C NMR for compounds **37/38**



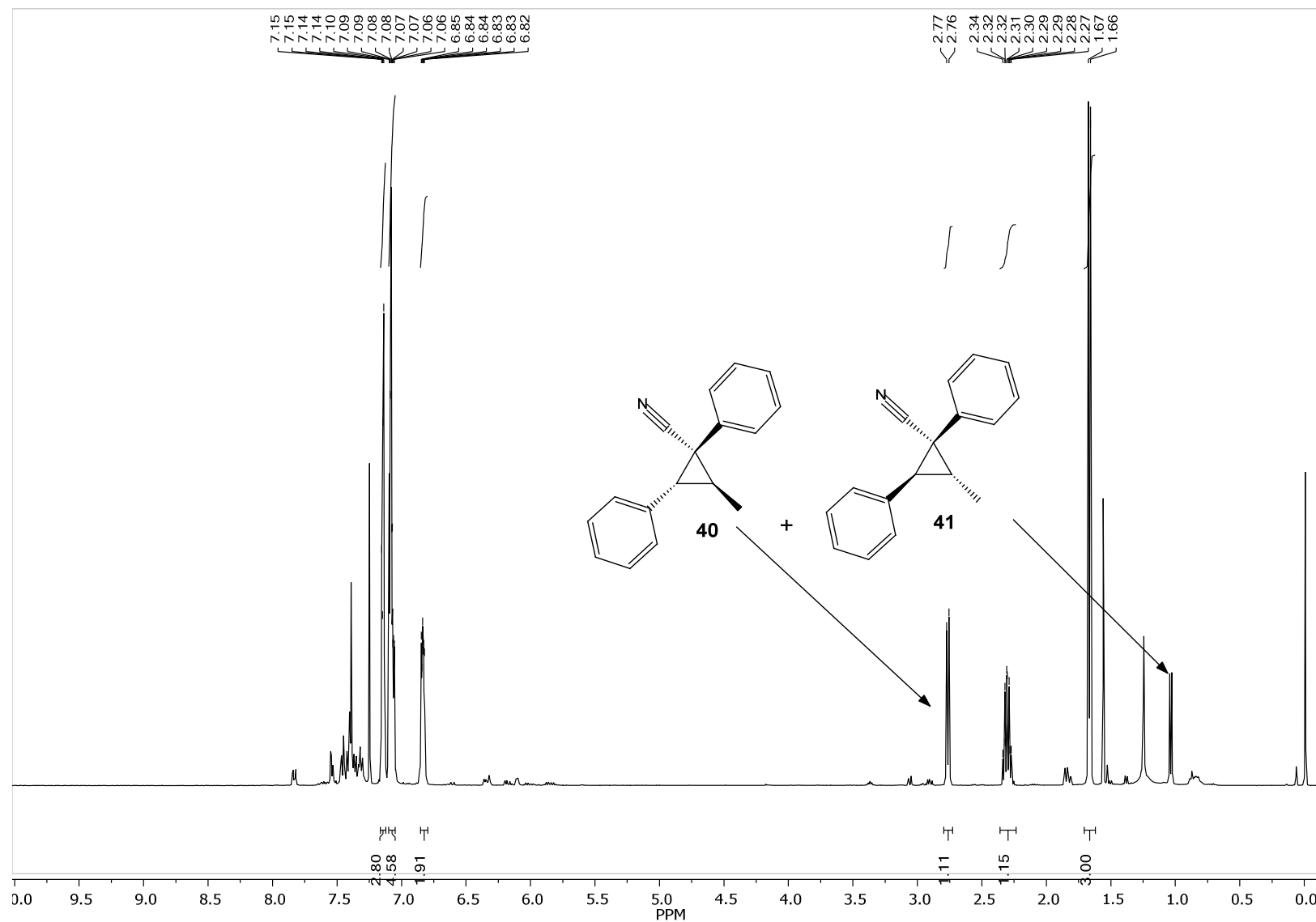
<sup>1</sup>H NMR for compound **39** (*exo* and *endo*-isomers)



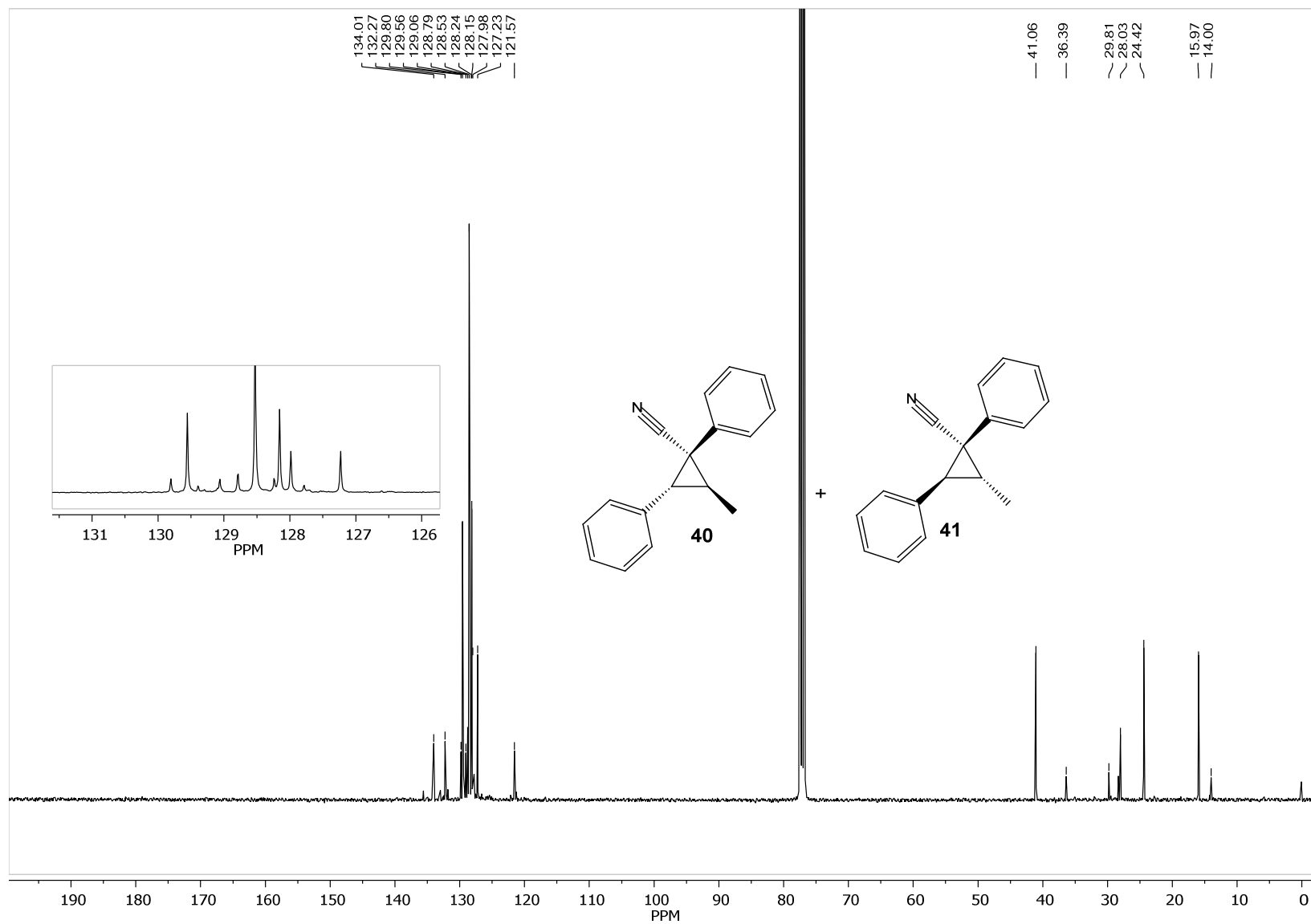
<sup>13</sup>C NMR for compound **39** (*exo* and *endo*-isomers)



<sup>1</sup>H NMR for compounds **40/41**

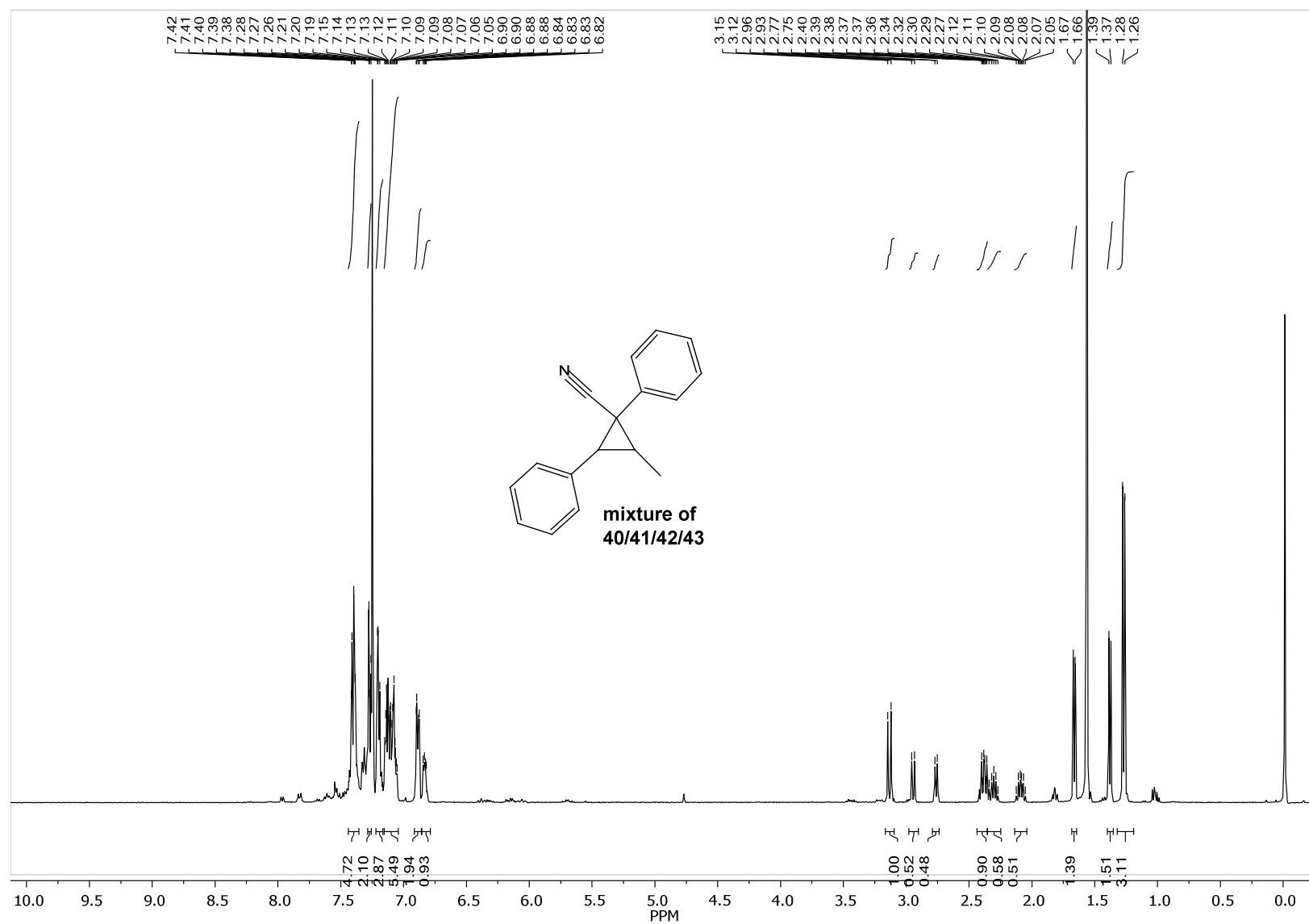


<sup>13</sup>C NMR for compounds **40/41**

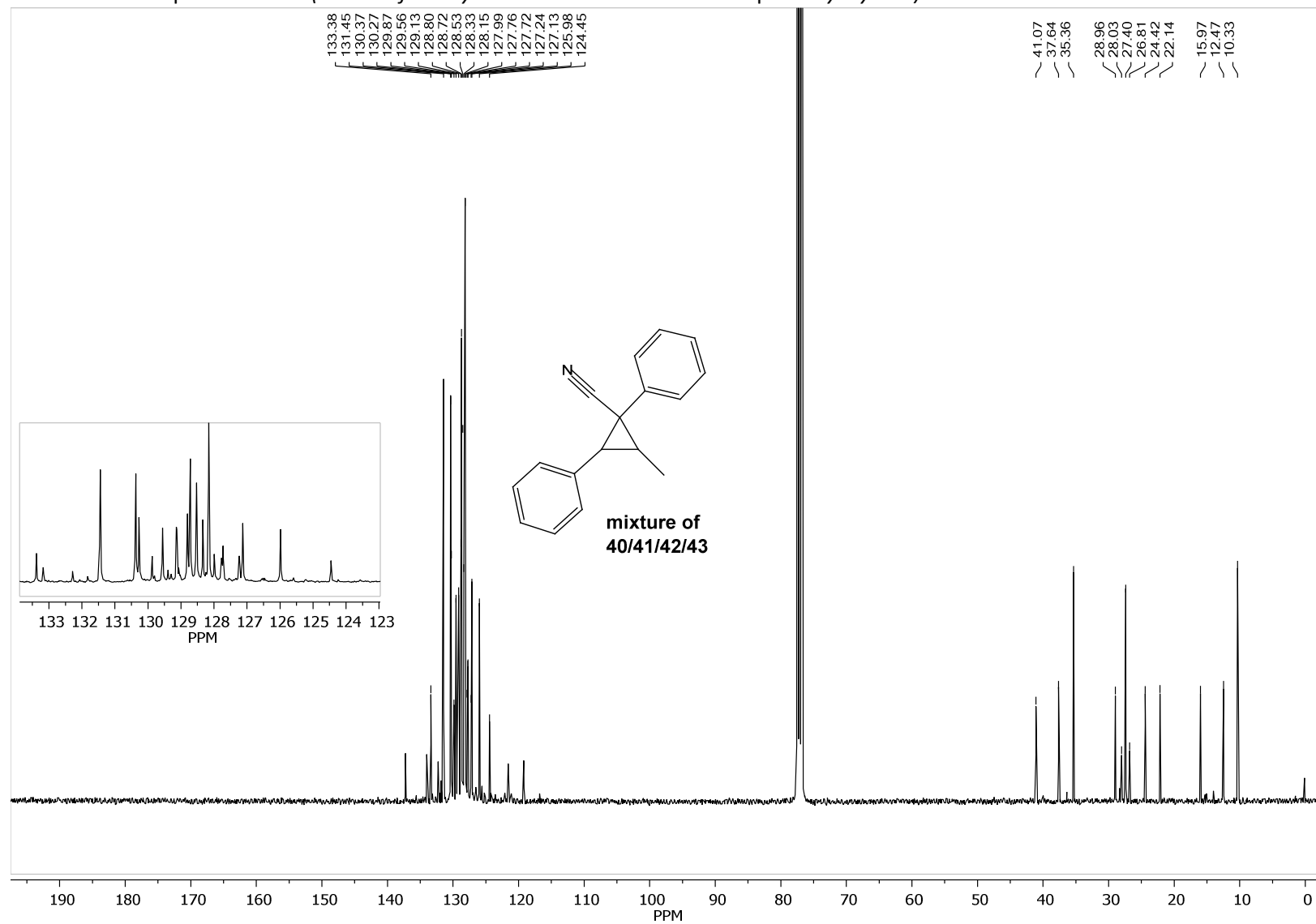




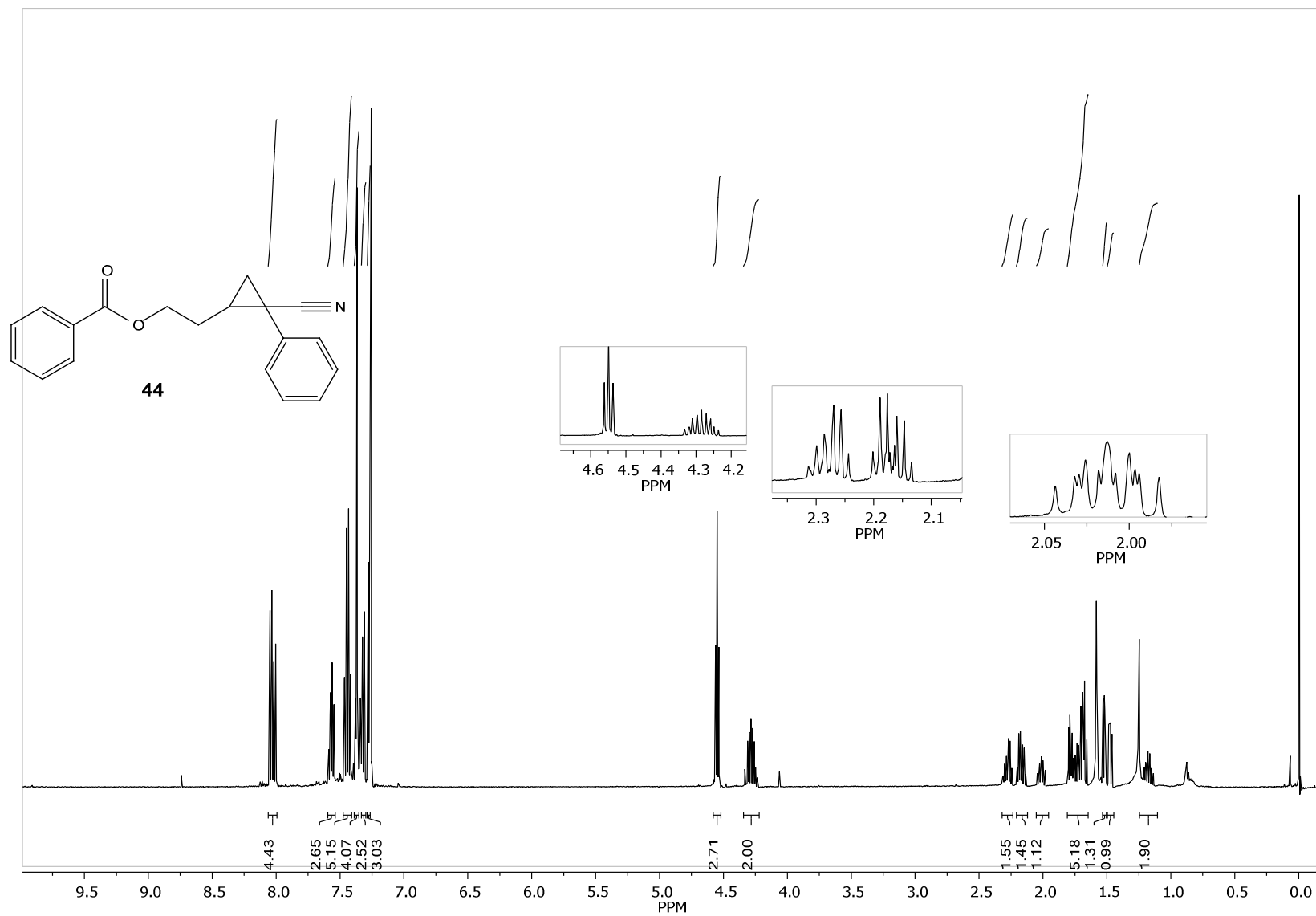
$^1\text{H}$  NMR for compounds **40-43** (isolated from cyanocarbene reaction with *cis*- $\beta$ -methylstyrene)



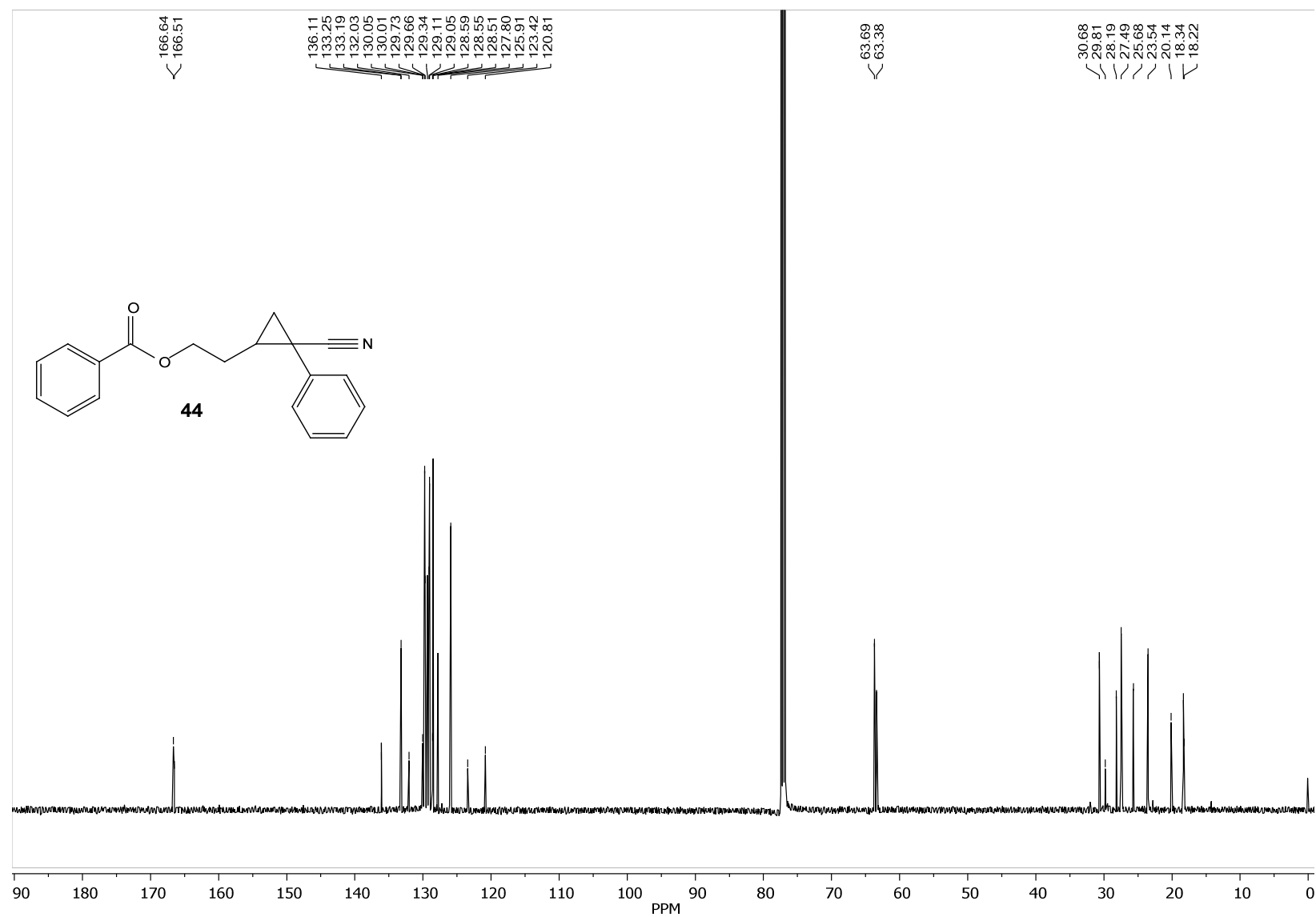
$^{13}\text{C}$  NMR for compounds **40-43** (isolated from cyanocarbene reaction with *cis*- $\beta$ -methylstyrene)



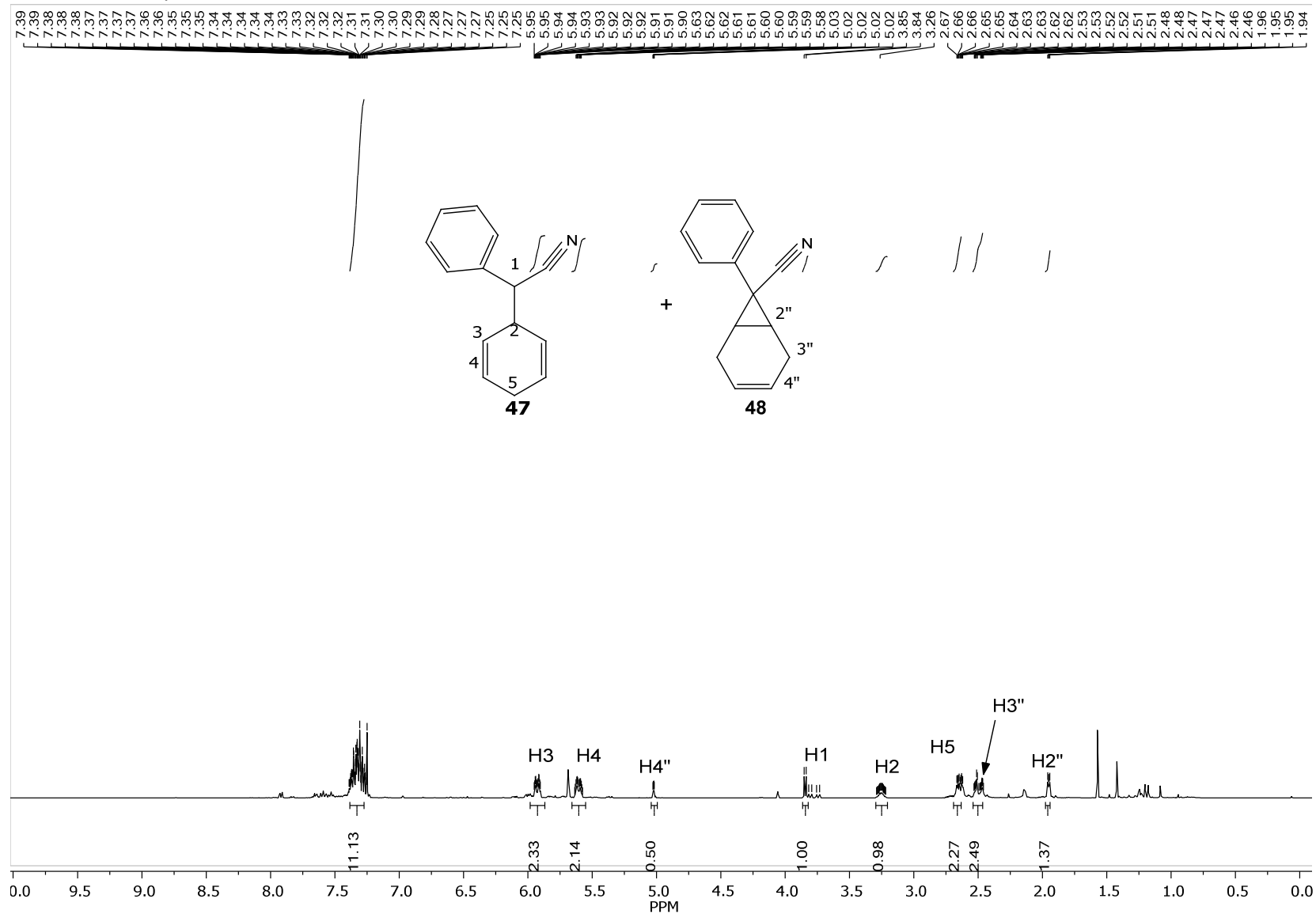
<sup>1</sup>H NMR for compound **44**



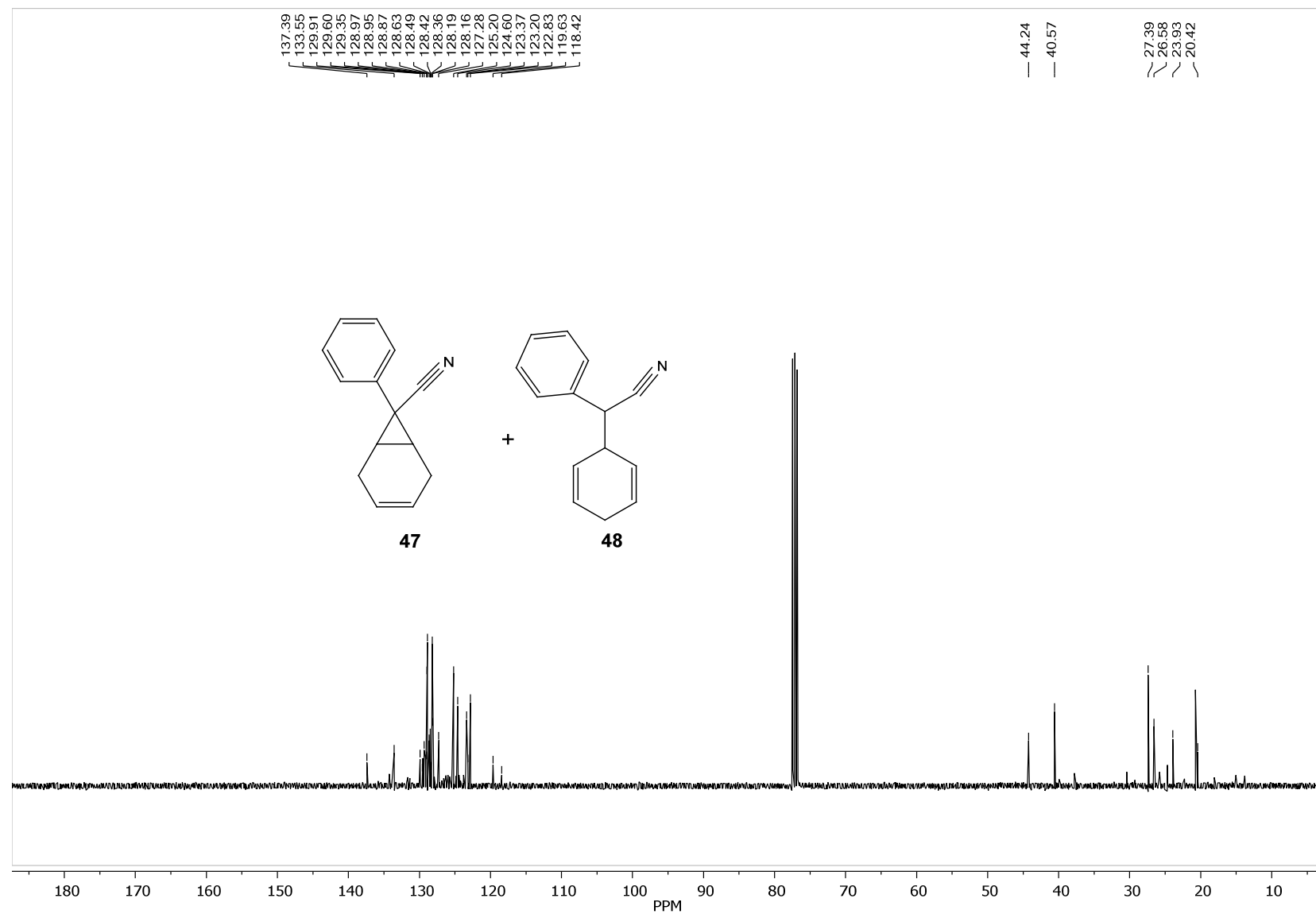
<sup>13</sup>C NMR for compound **44**



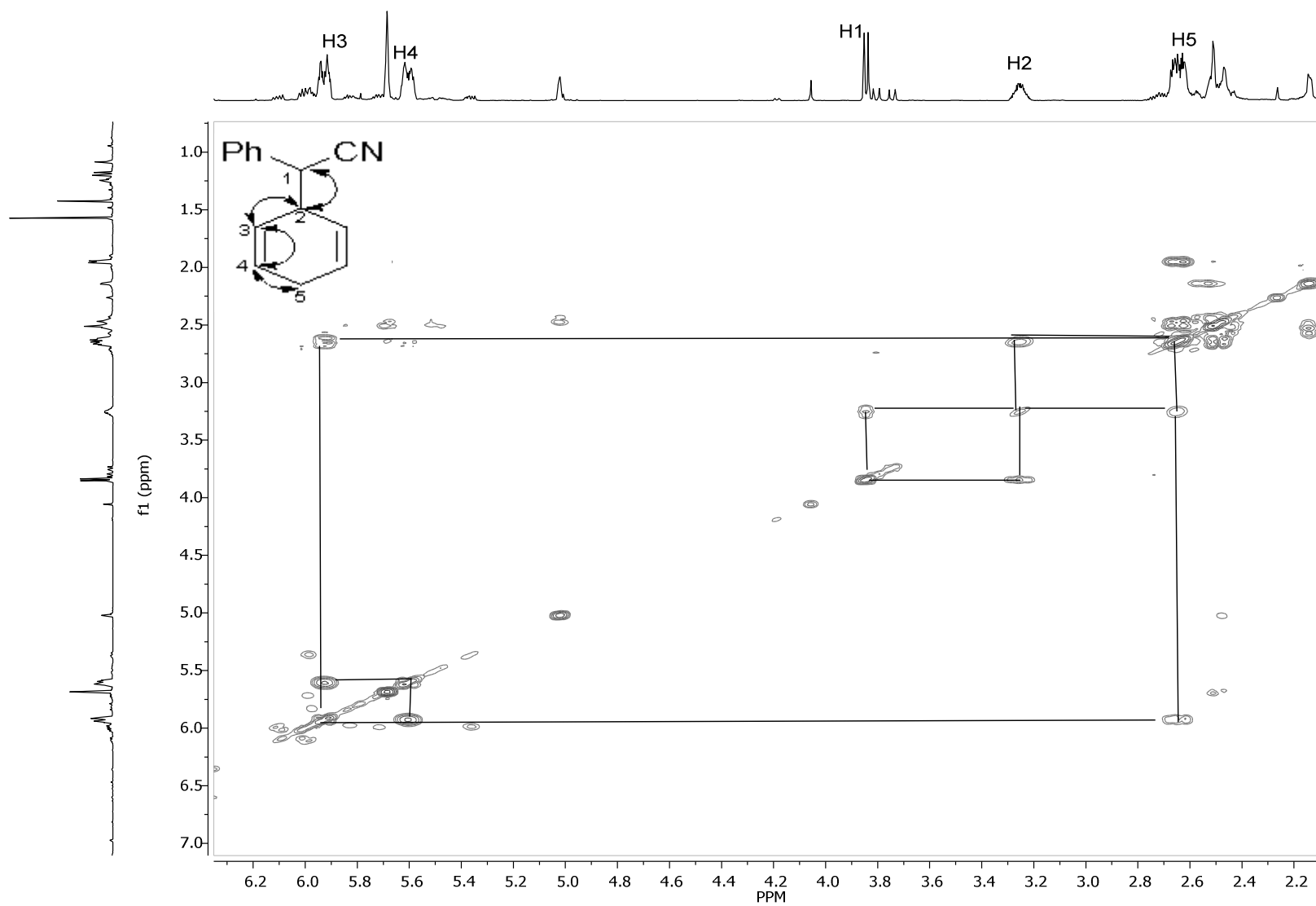
<sup>1</sup>H NMR for compounds **47/48**



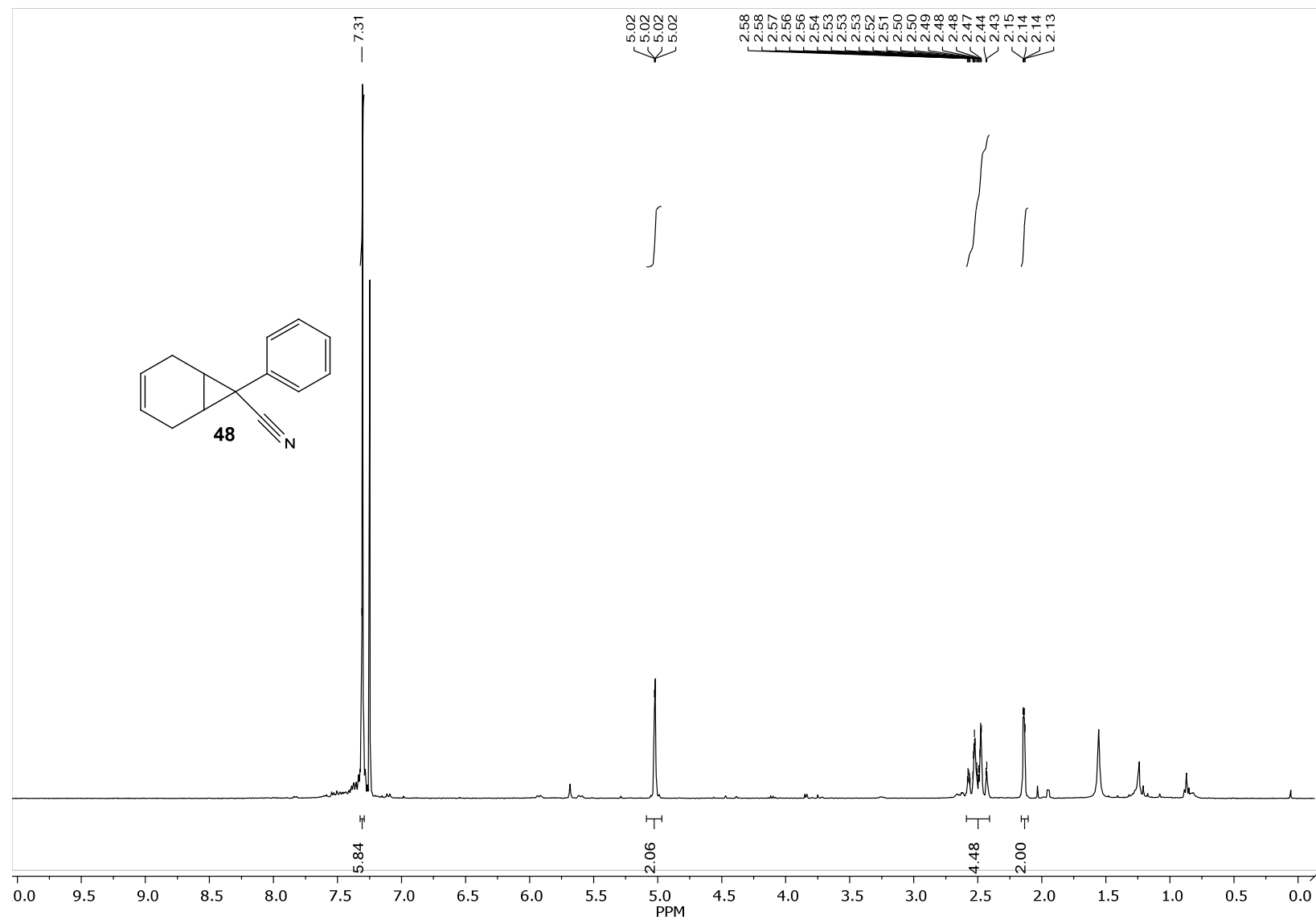
<sup>13</sup>C NMR for compounds **47/48**



$^1\text{H}$ - $^1\text{H}$  COSY for compounds **47/48**

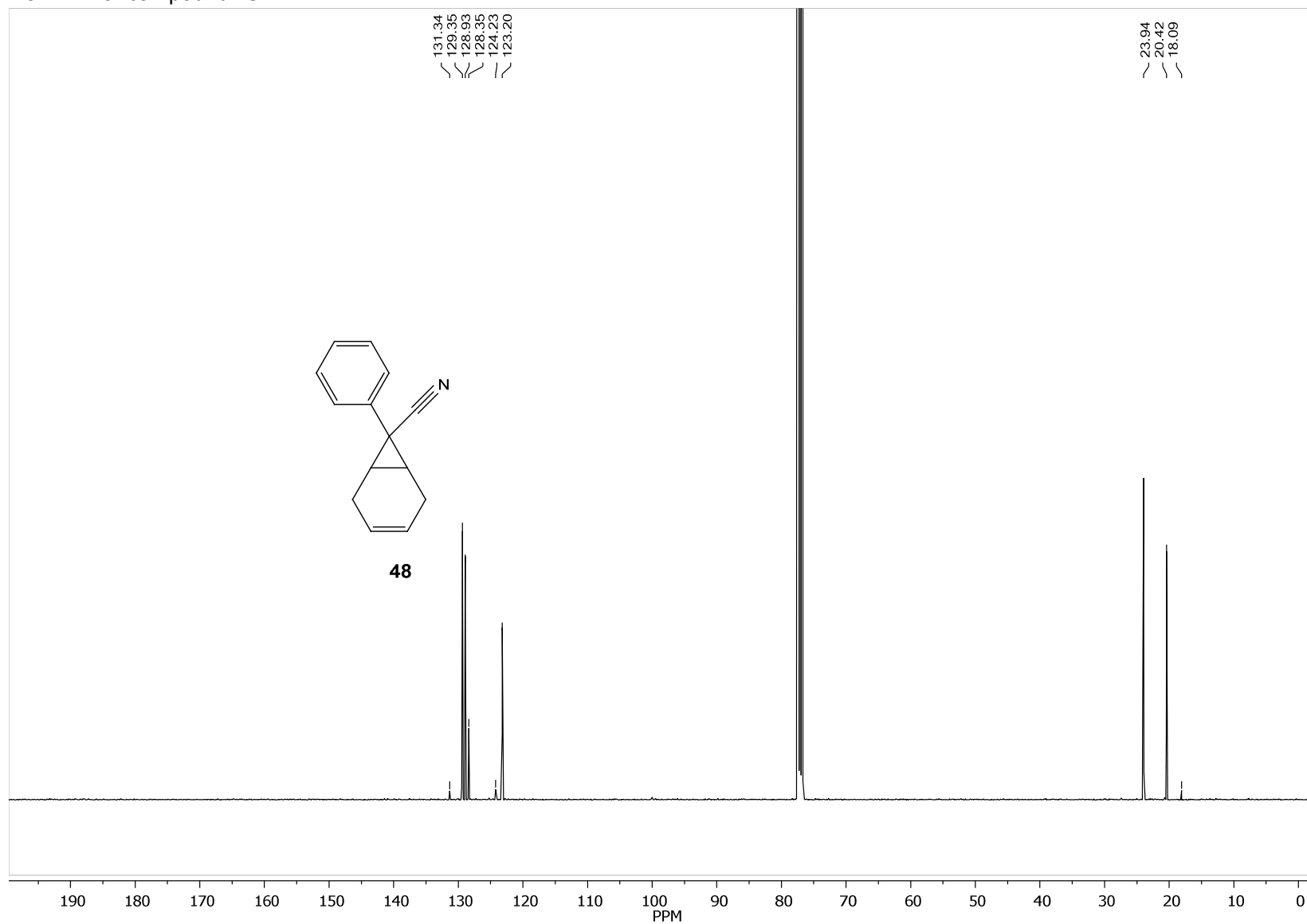


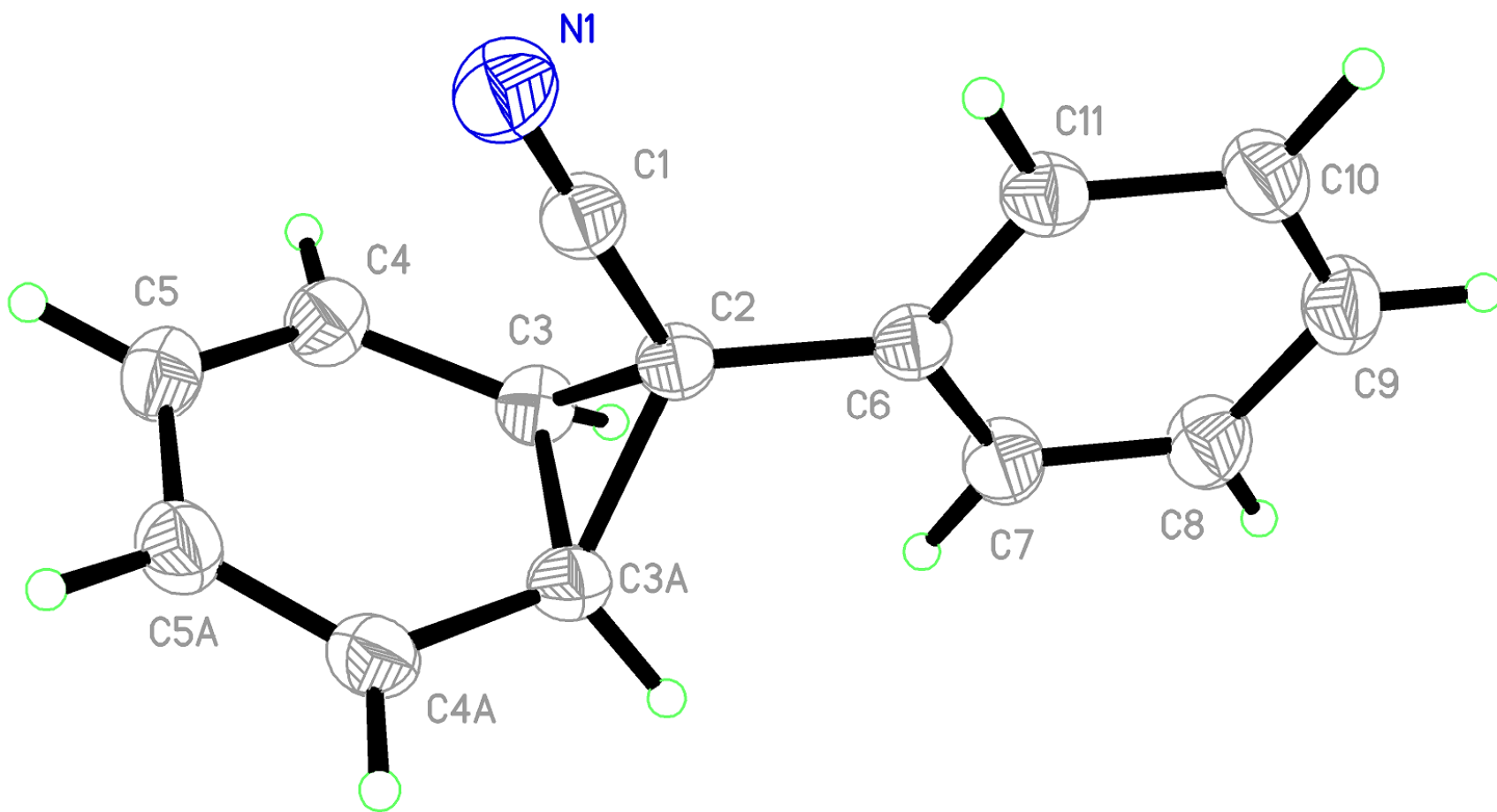
<sup>1</sup>H NMR for compounds **48**



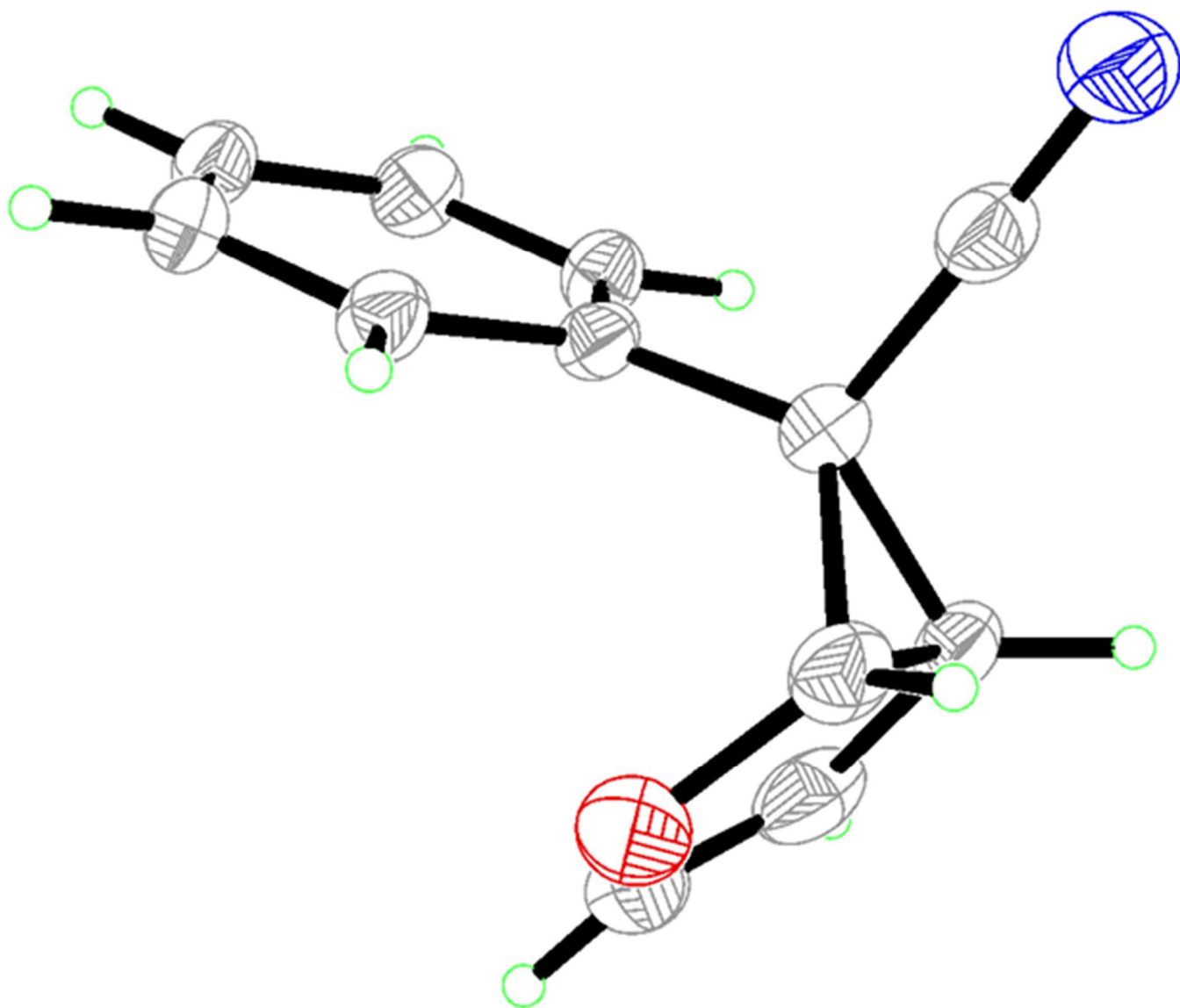


<sup>13</sup>C NMR for compound **48**





X-ray structure ORTEP diagram of compound **13**. Thermal ellipsoids are set to 50% probability level



X-ray structure ORTEP diagram of compound **32**. Thermal ellipsoids are set to 50% probability level