

## **Supplementary Information**

# **Synthesis and antiproliferative activity of phosphorus substituted 4-cyanooxazolines, 2-aminocyanooxazolines, 2-iminocyanooxazolidines, and 2-aminocyanothiazolines by rearrangement of cyanoaziridines**

**Victor Carramiñana, Ana M. Ochoa de Retana, Francisco Palacios\*, Jesús M. de los Santos\***

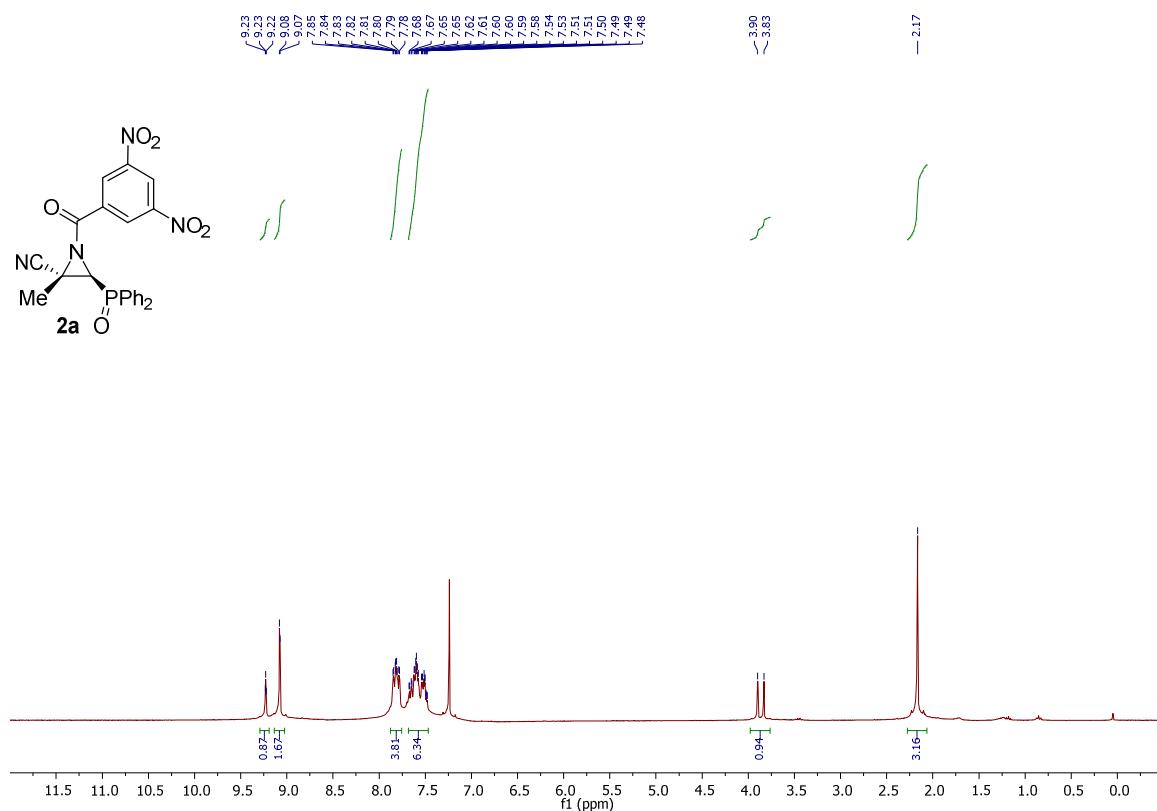
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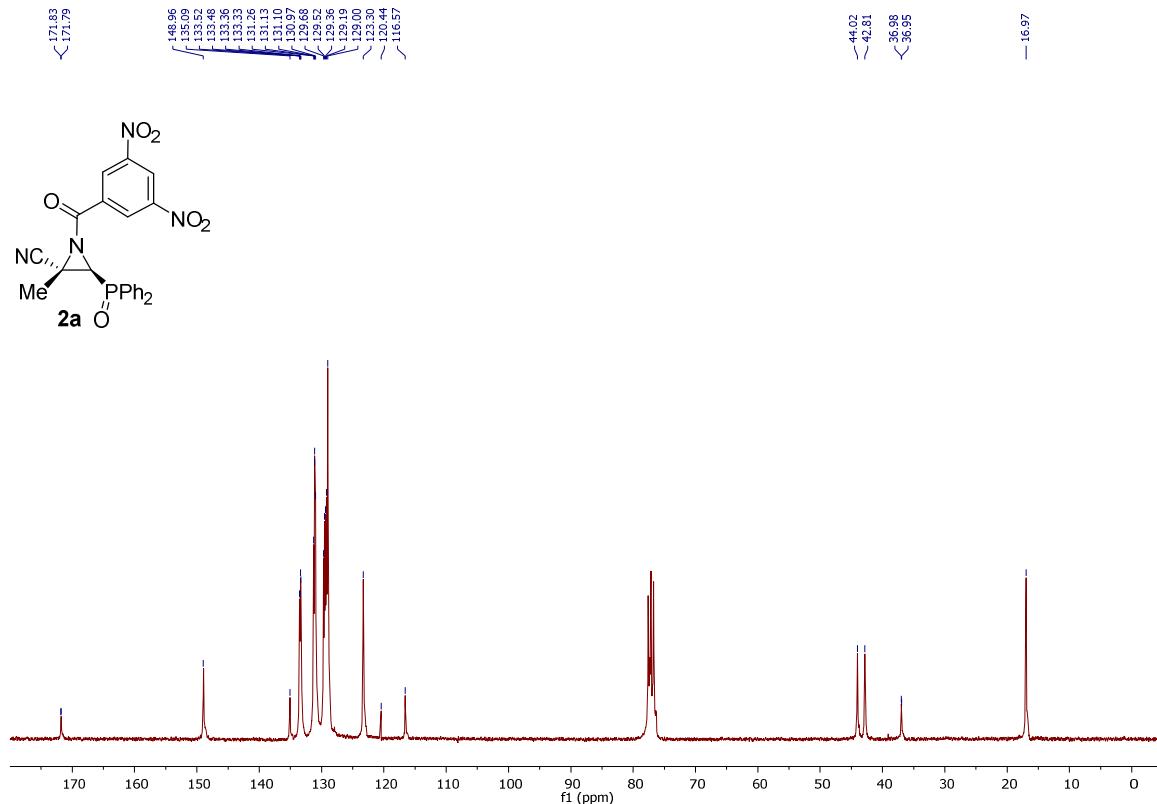
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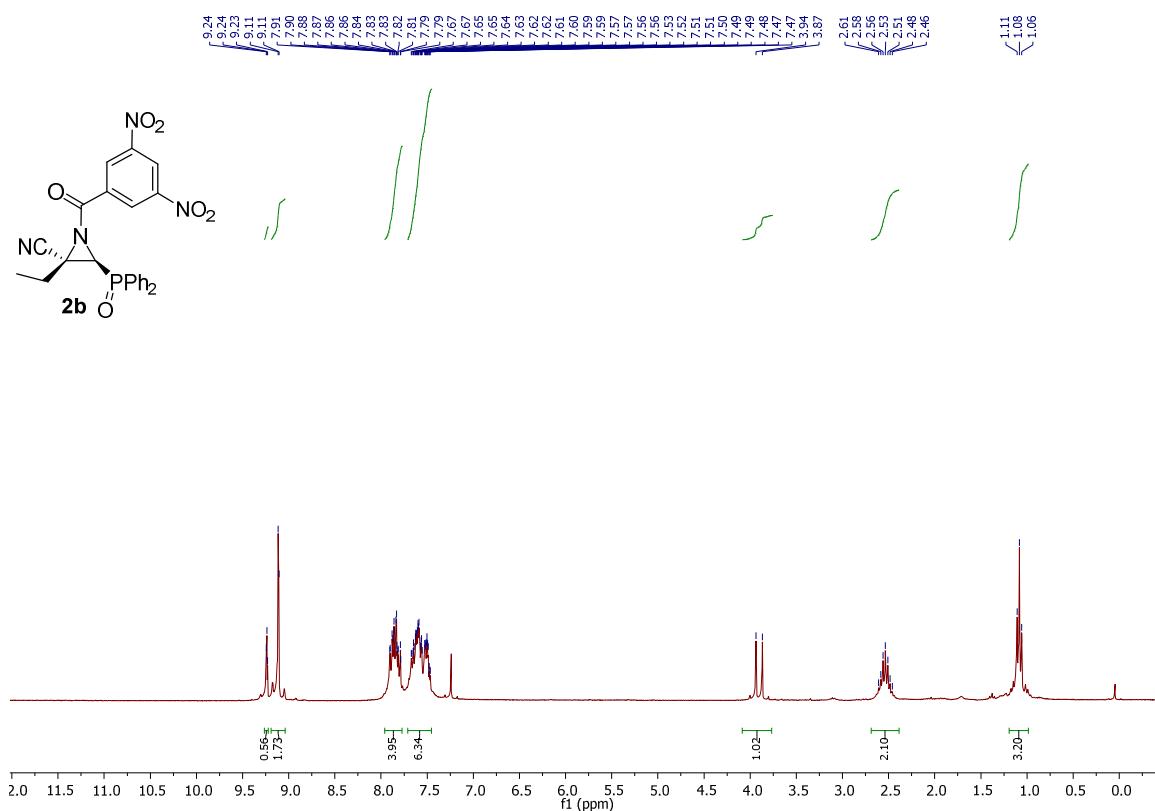
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound **2a**.



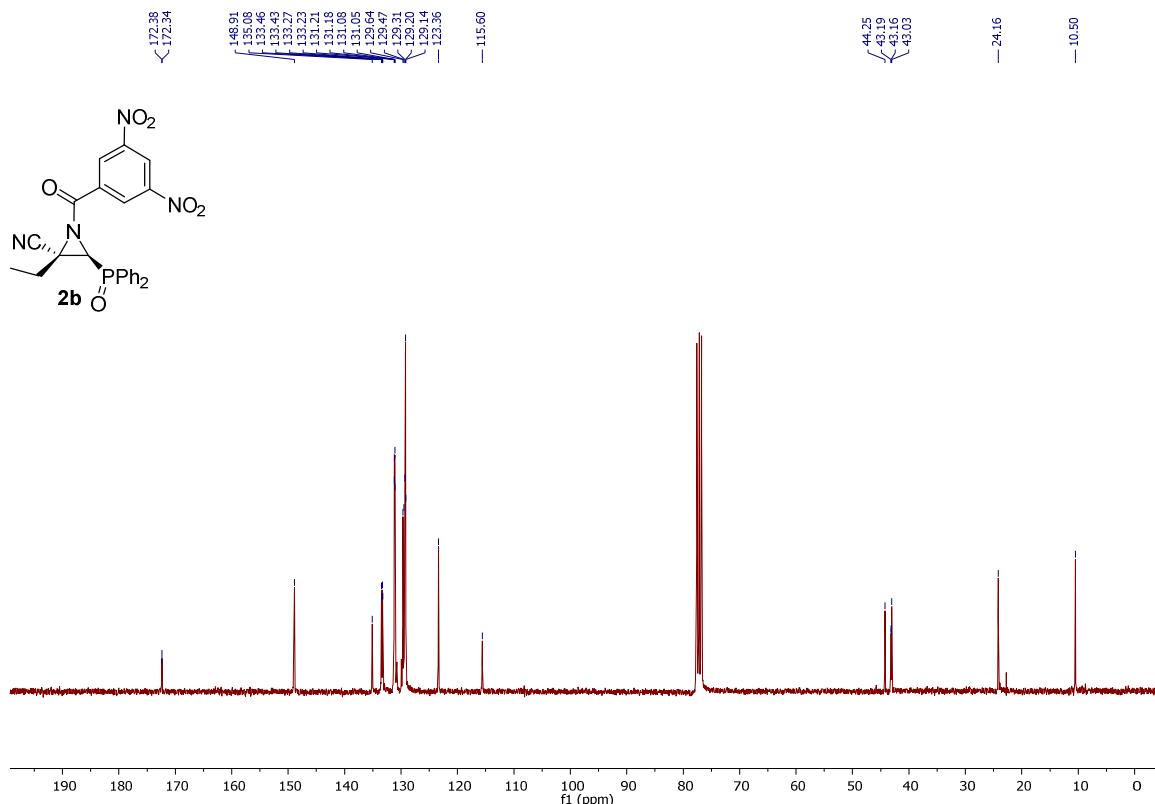
<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>) of compound **2a**.



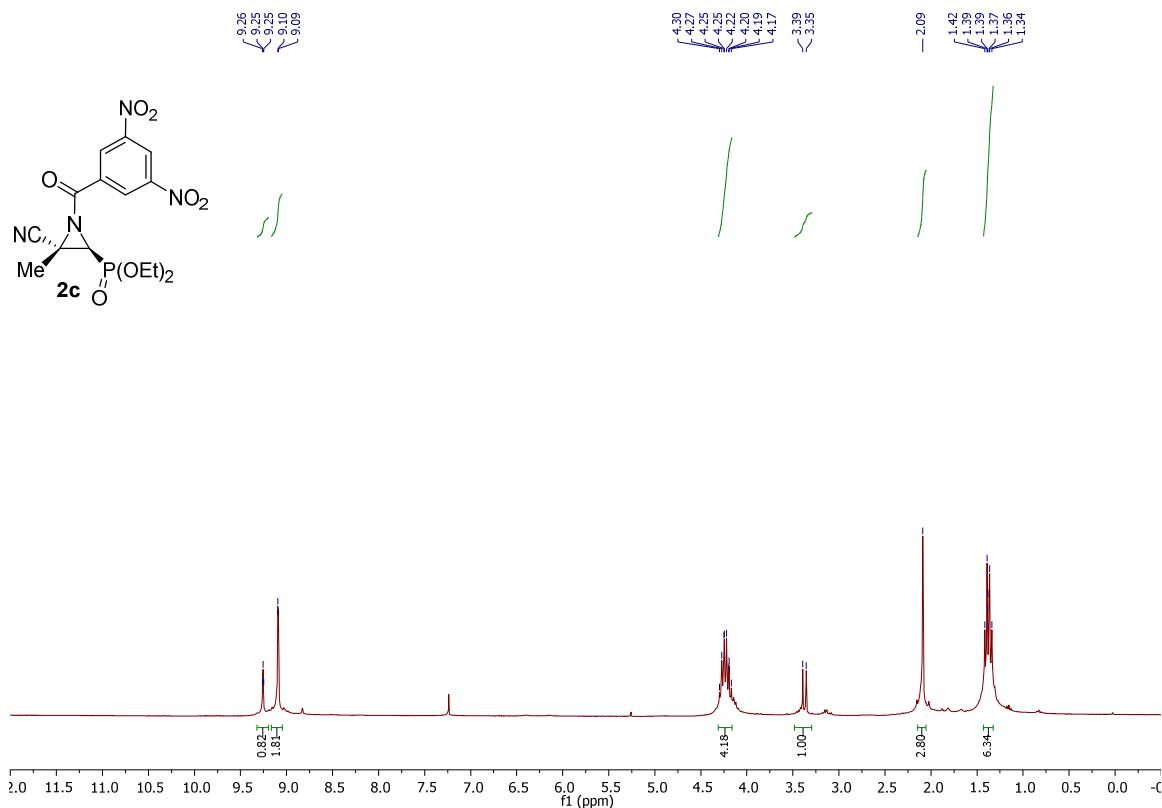
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound **2b**.



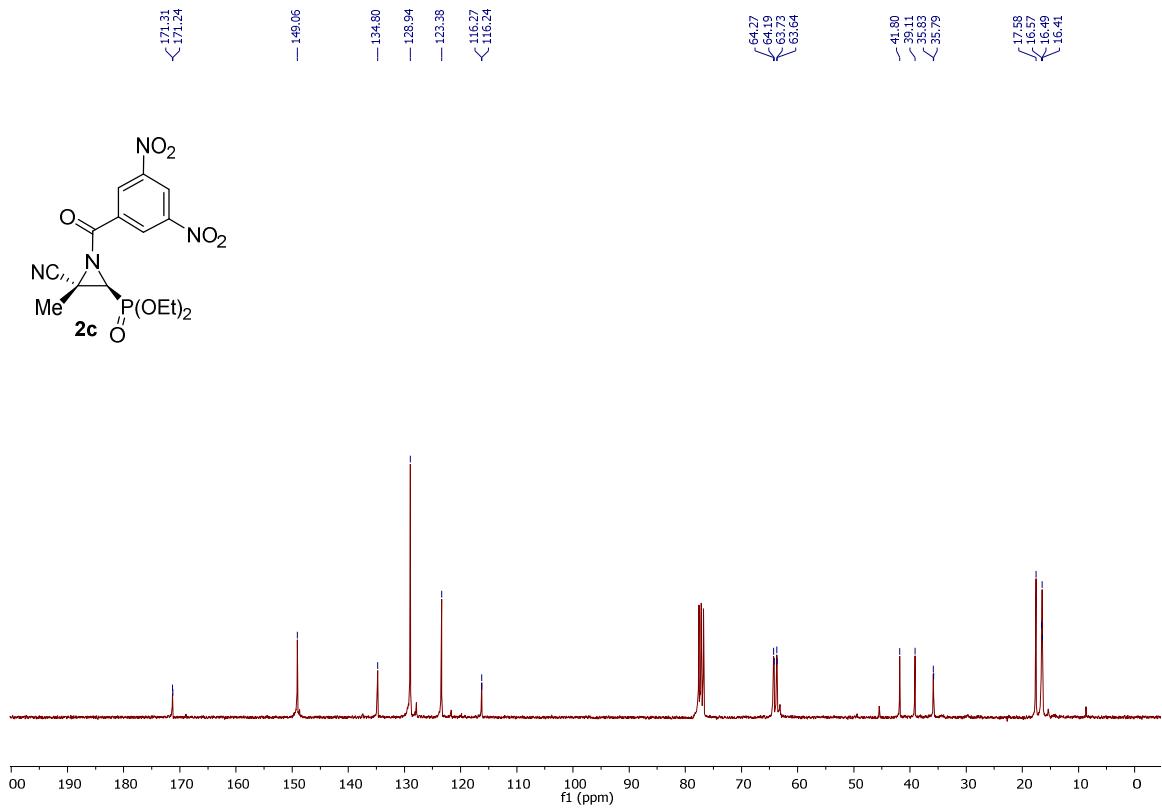
<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>) of compound **2b**.



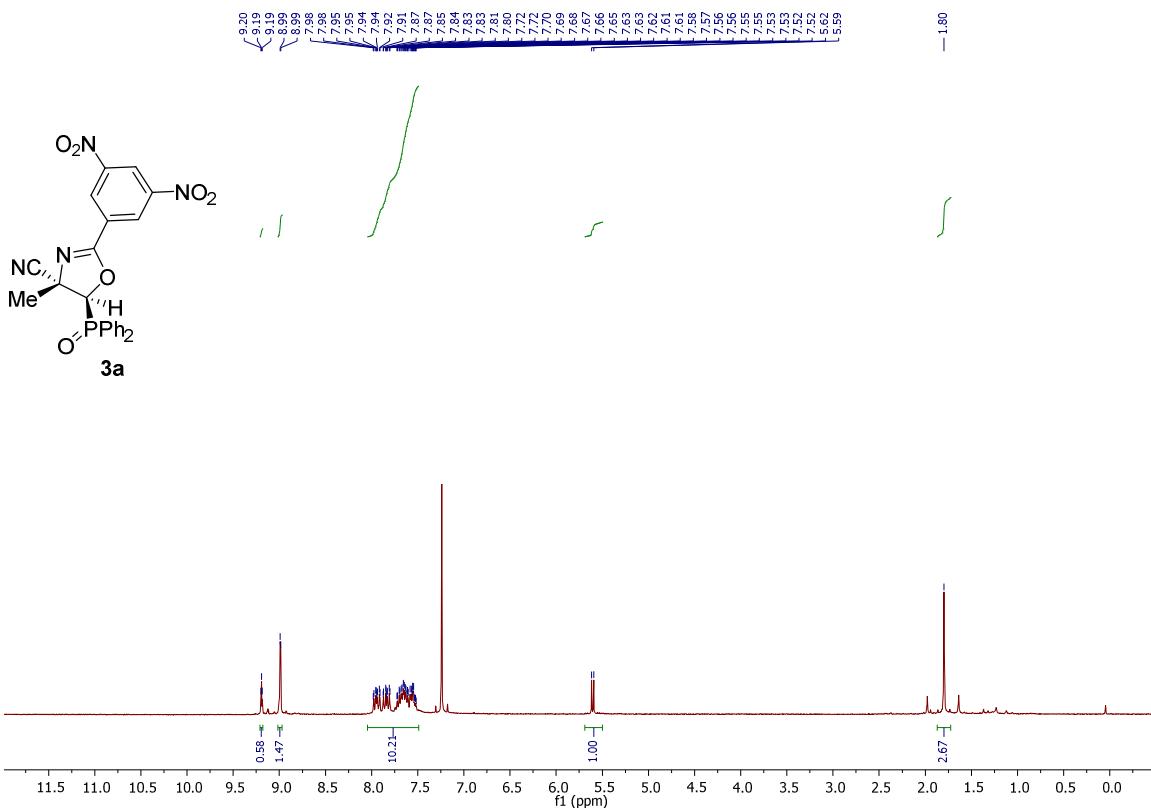
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound **2c**.



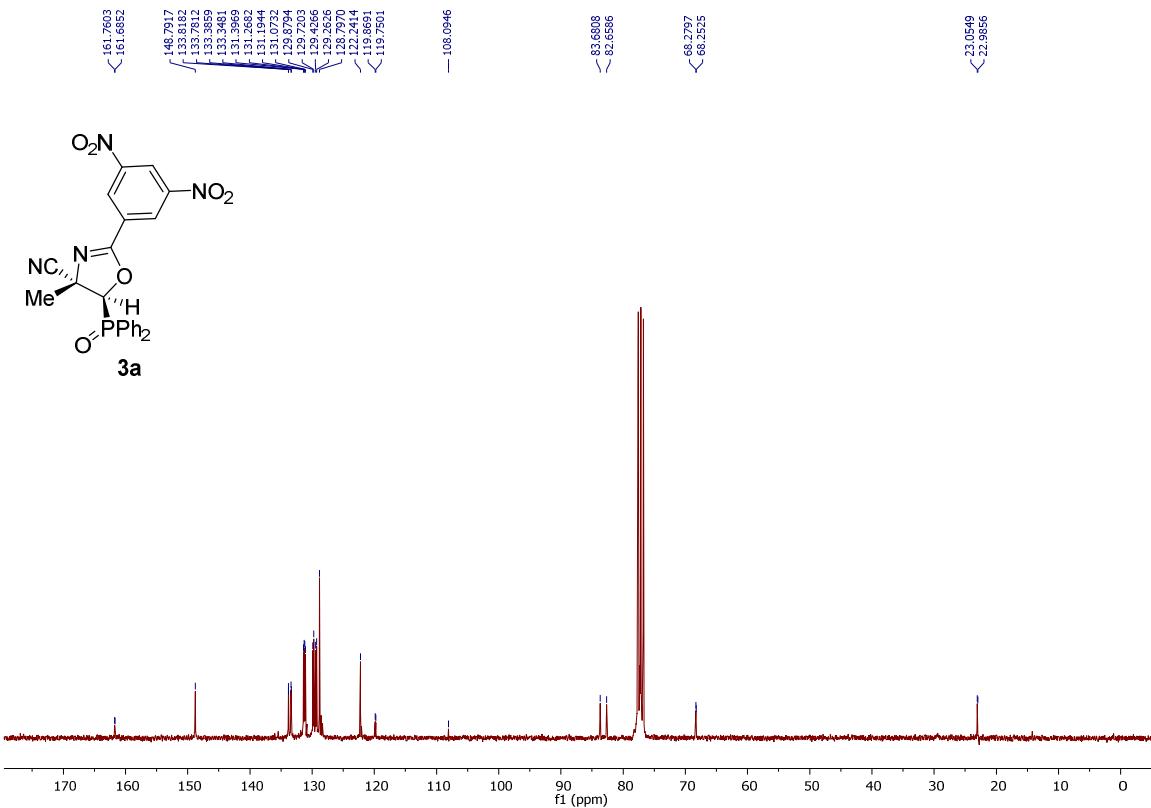
$^{13}\text{C}$  { $^1\text{H}$ } NMR (75 MHz,  $\text{CDCl}_3$ ) of compound **2c**.



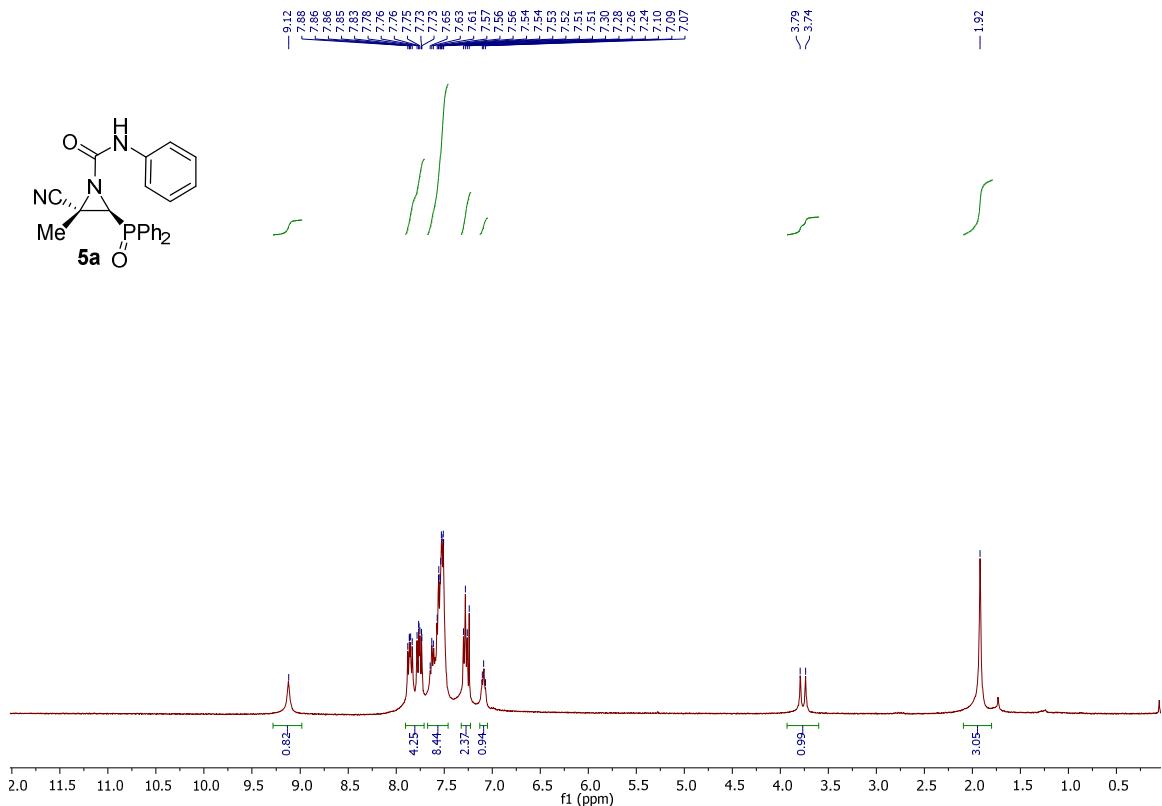
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 3a.



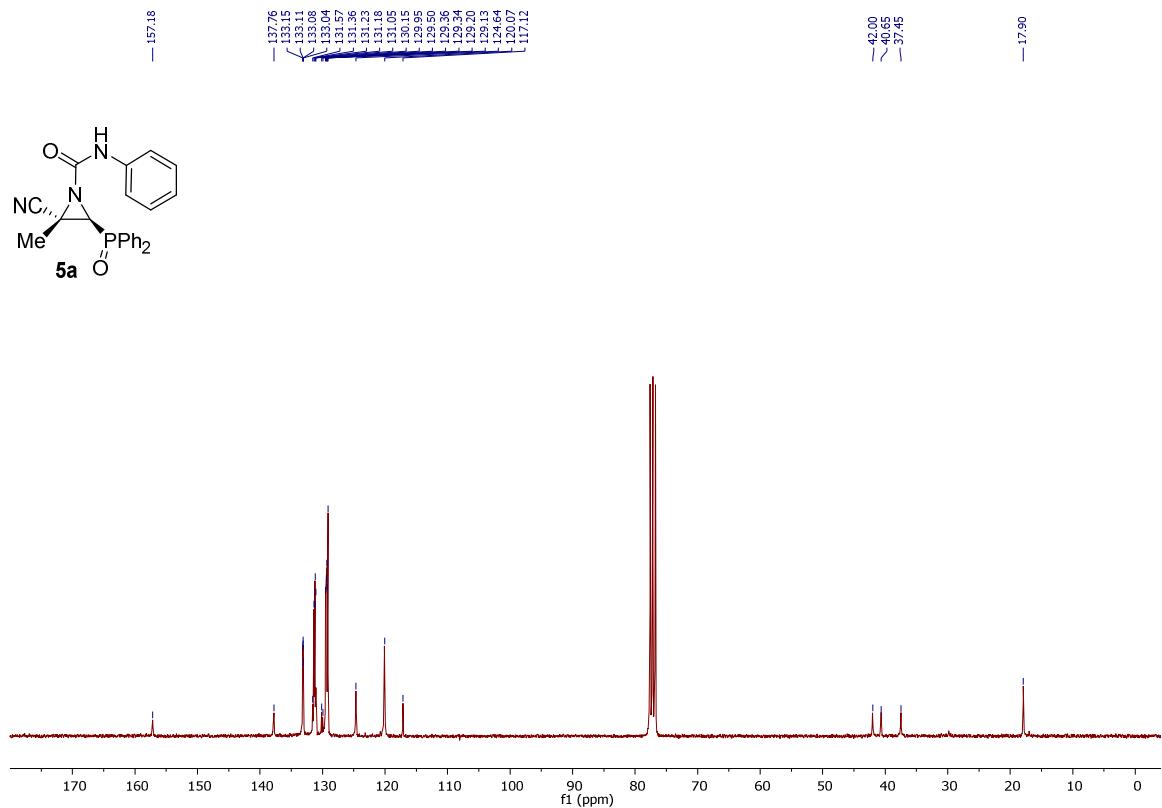
<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>) of compound 3a.



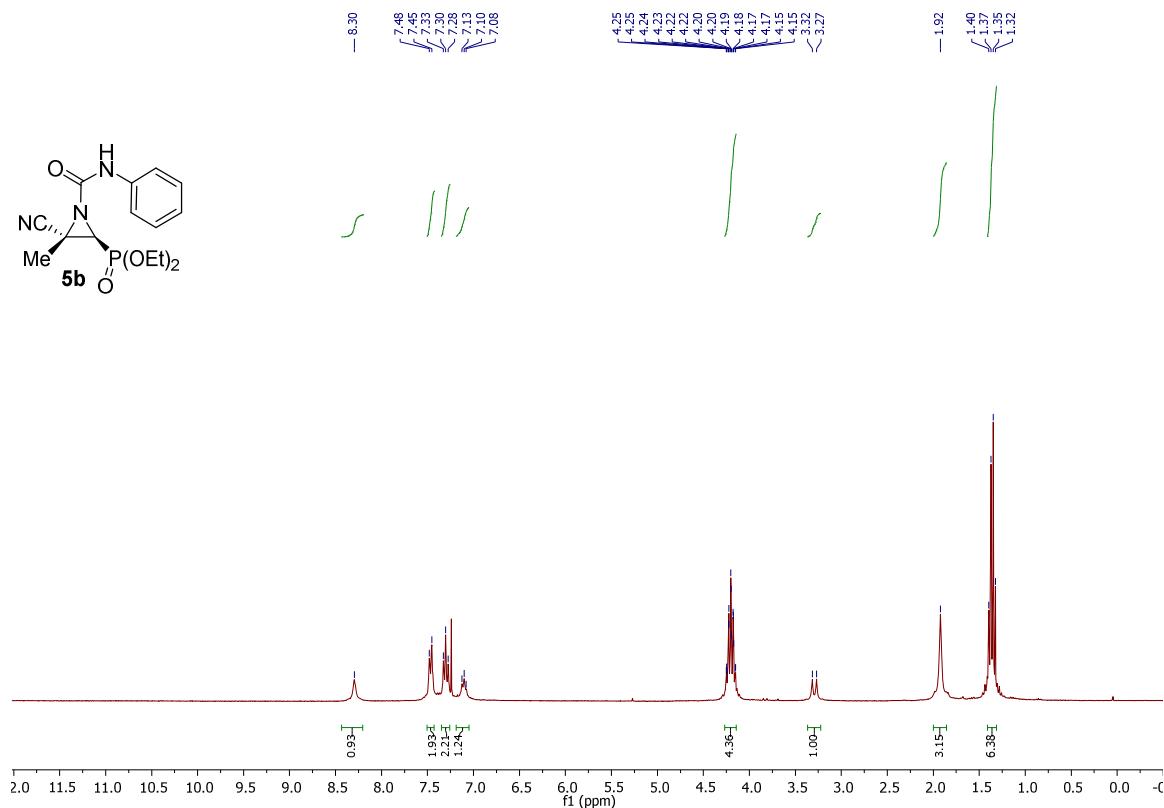
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **5a**.



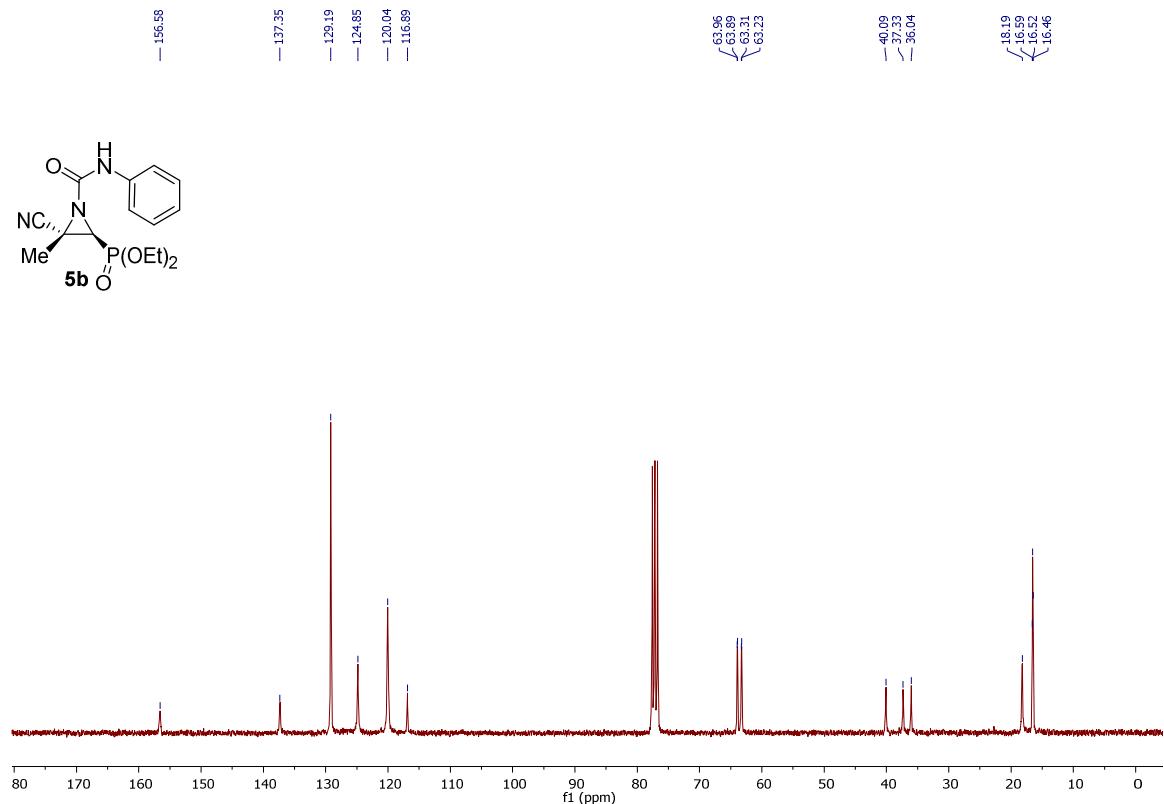
<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of compound **5a**.



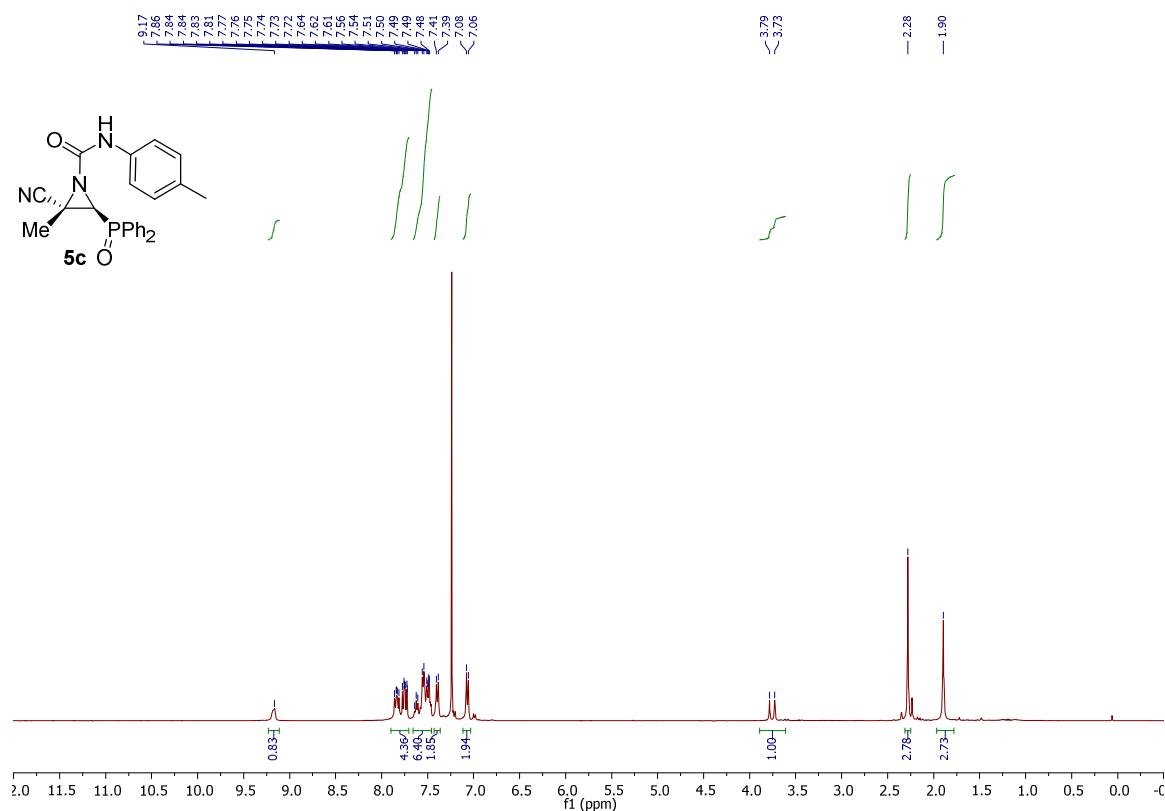
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) of compound **5b**.



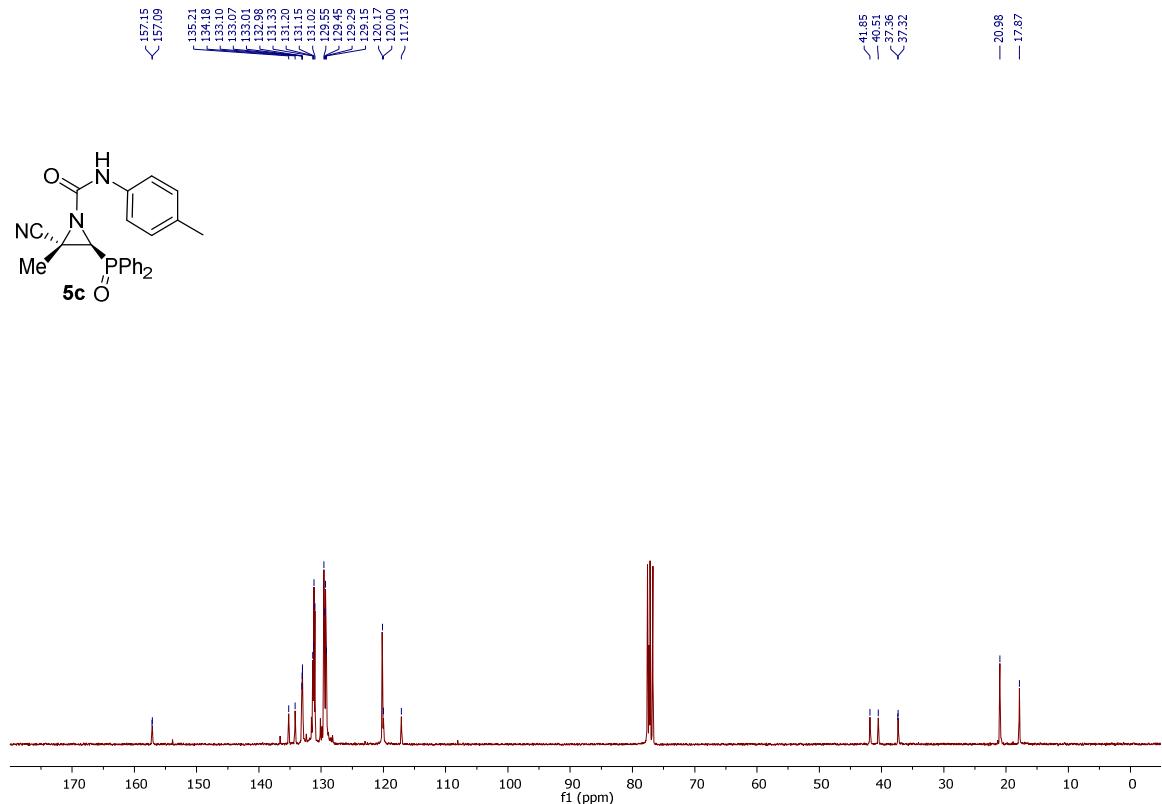
$^{13}\text{C}\{^1\text{H}\}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound **5b**.



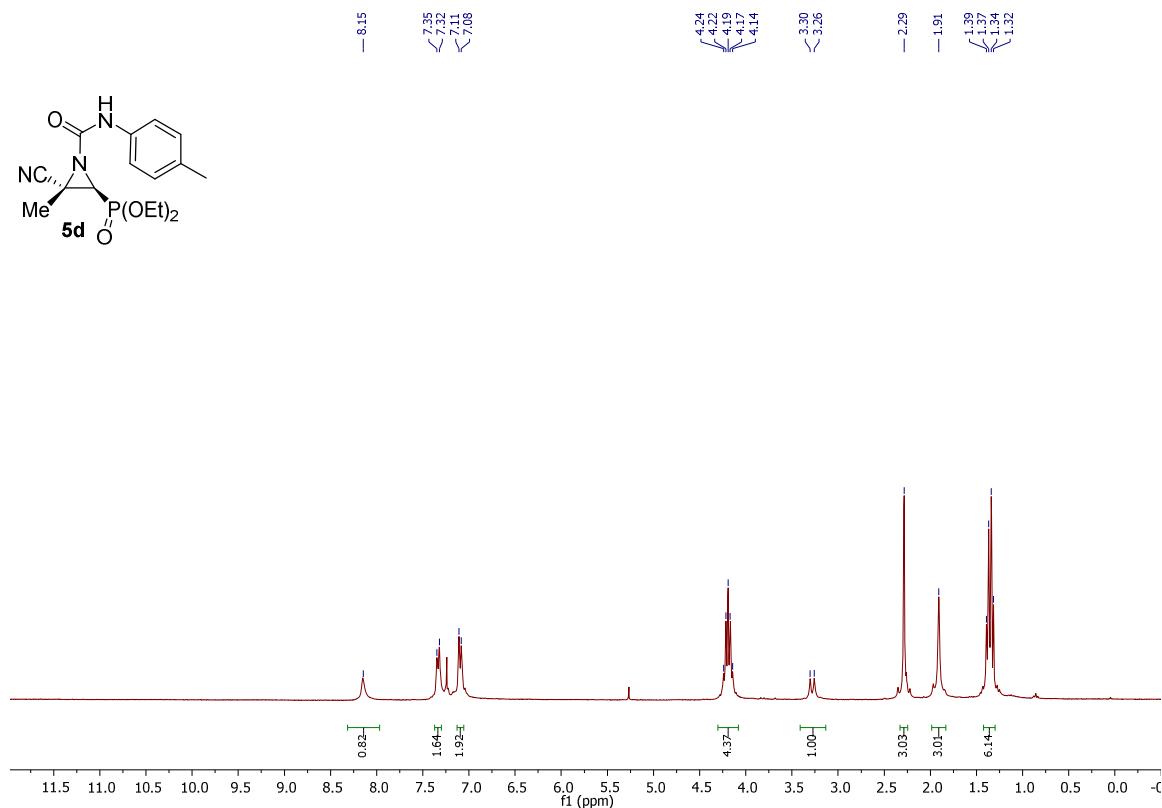
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound 5c.



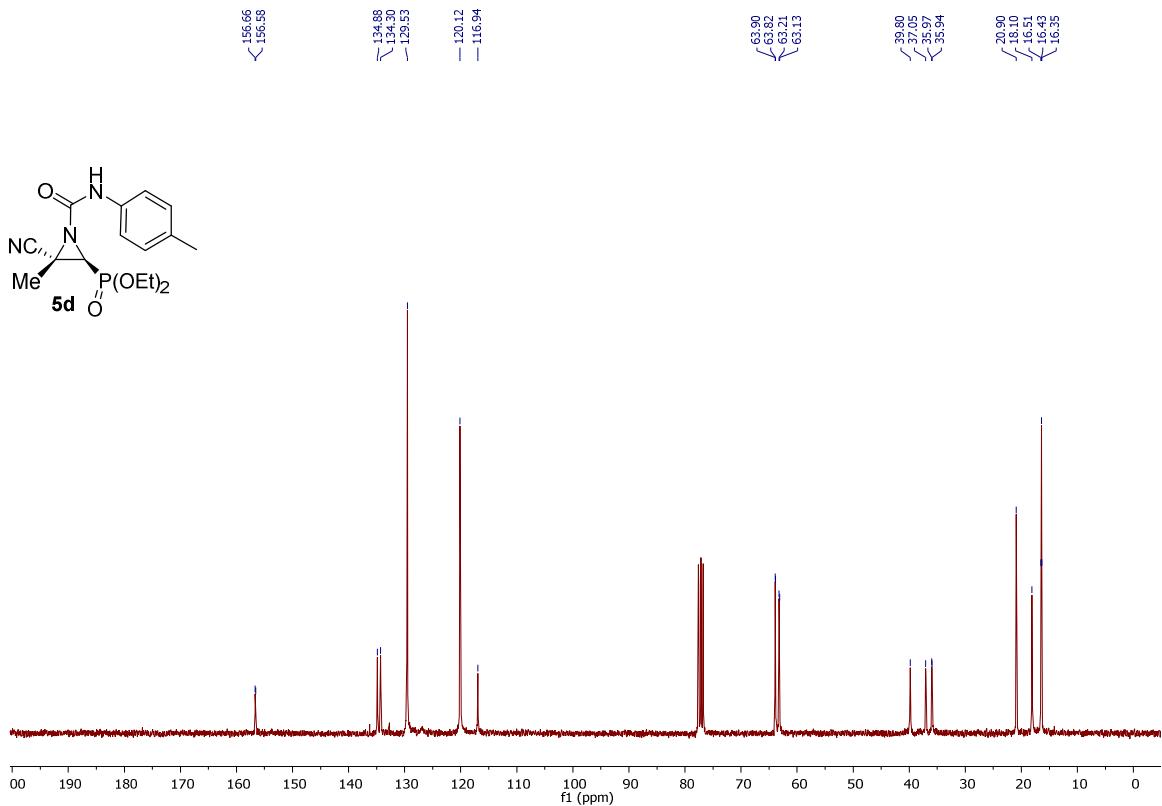
$^{13}\text{C}$  { $^1\text{H}$ } NMR (75 MHz,  $\text{CDCl}_3$ ) of compound **5c**.



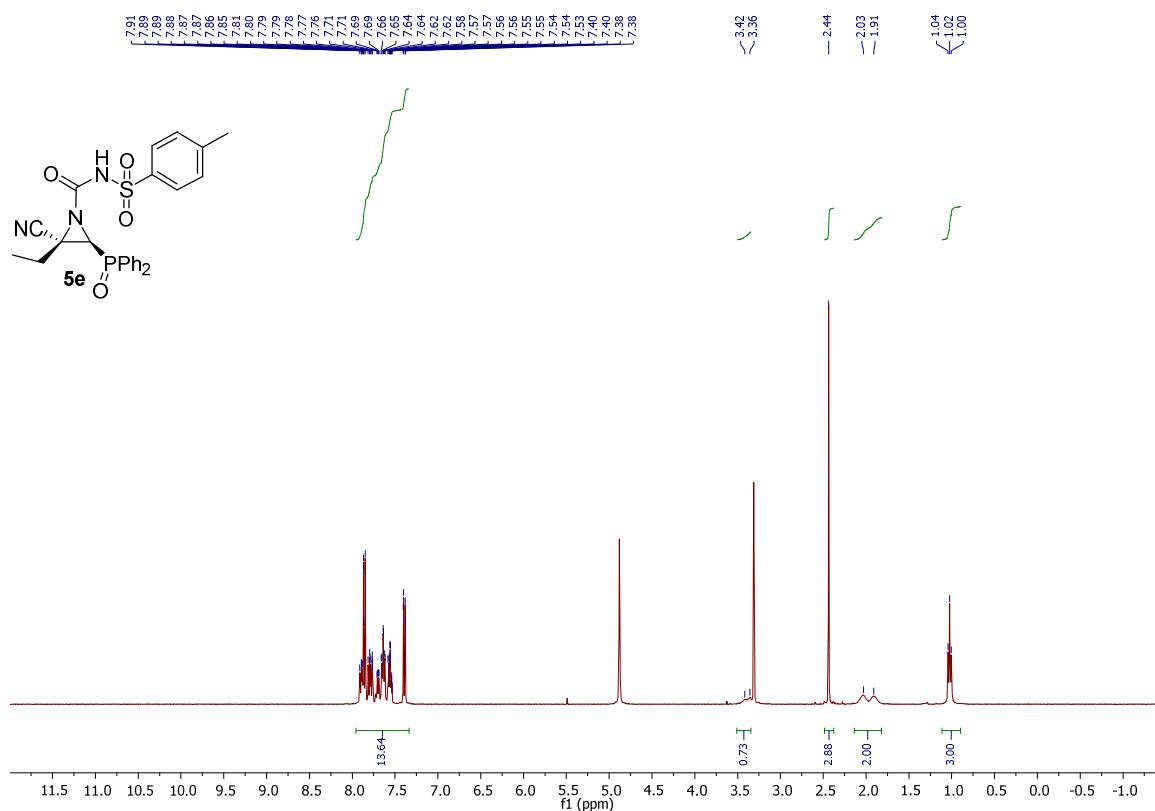
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound **5d**.



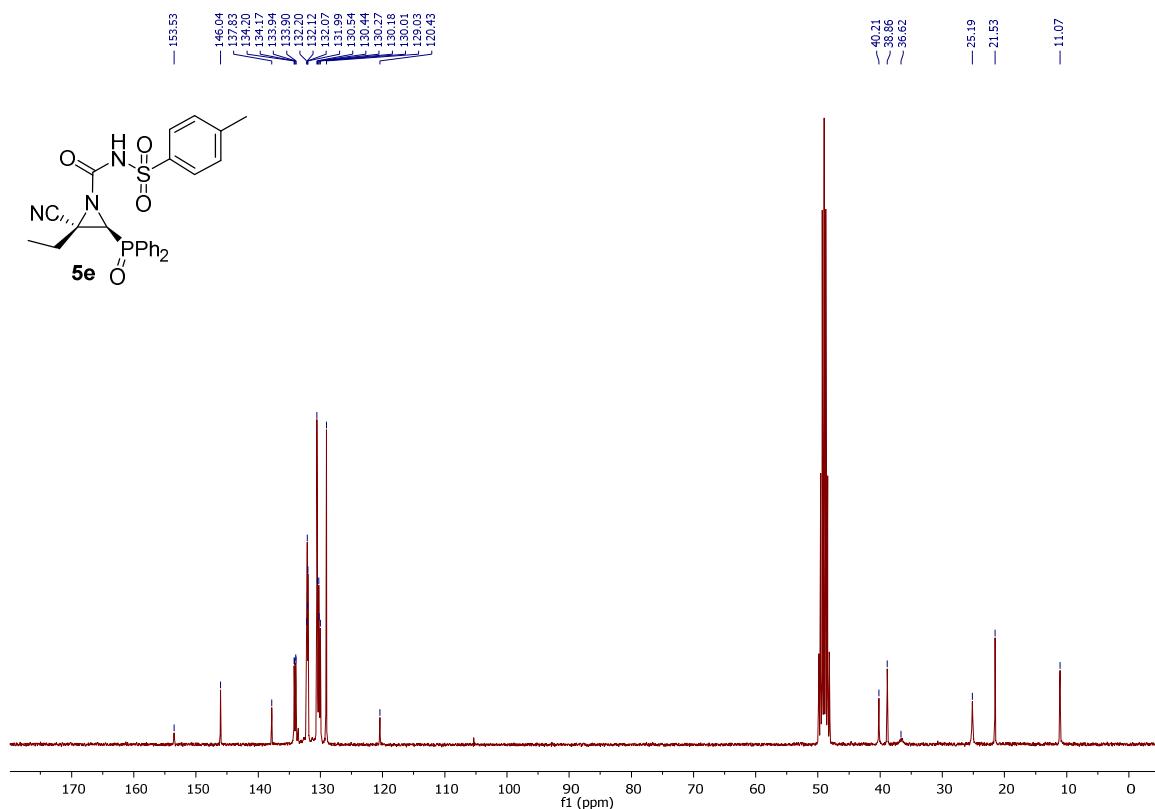
<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>) of compound **5d**.



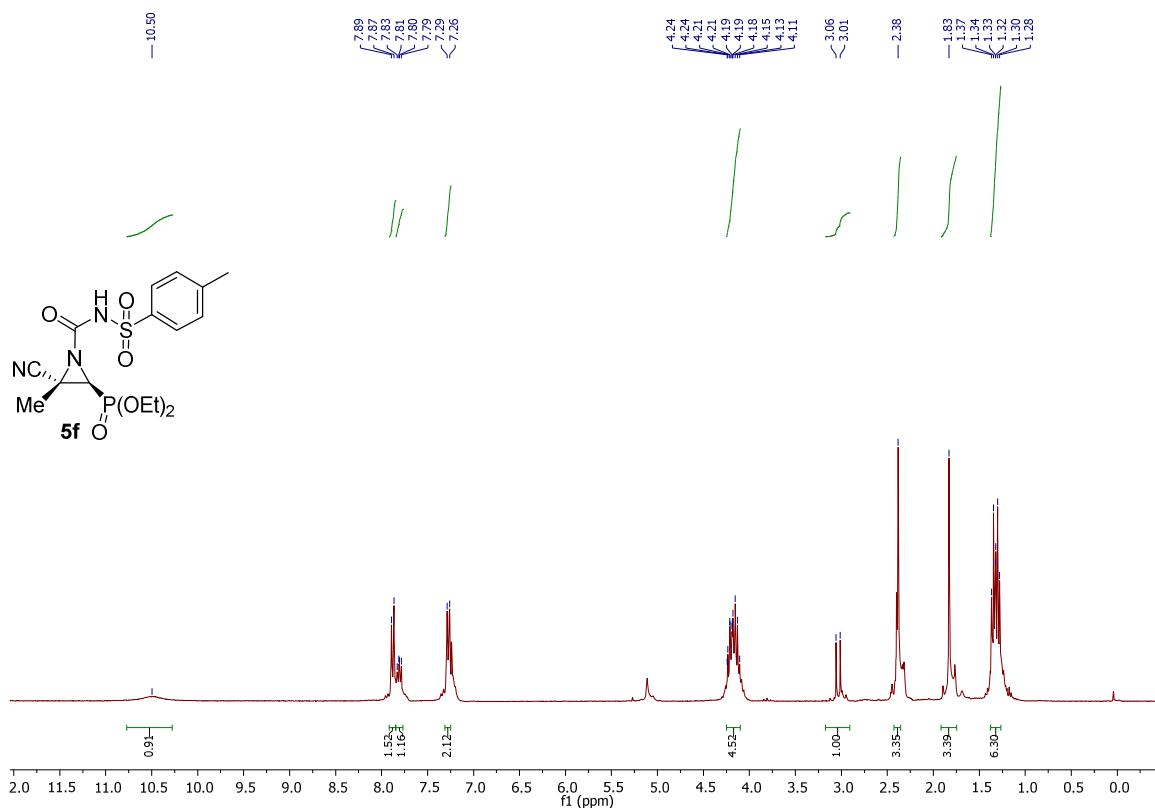
<sup>1</sup>H NMR (400 MHz, MeOD) of compound **5e**.



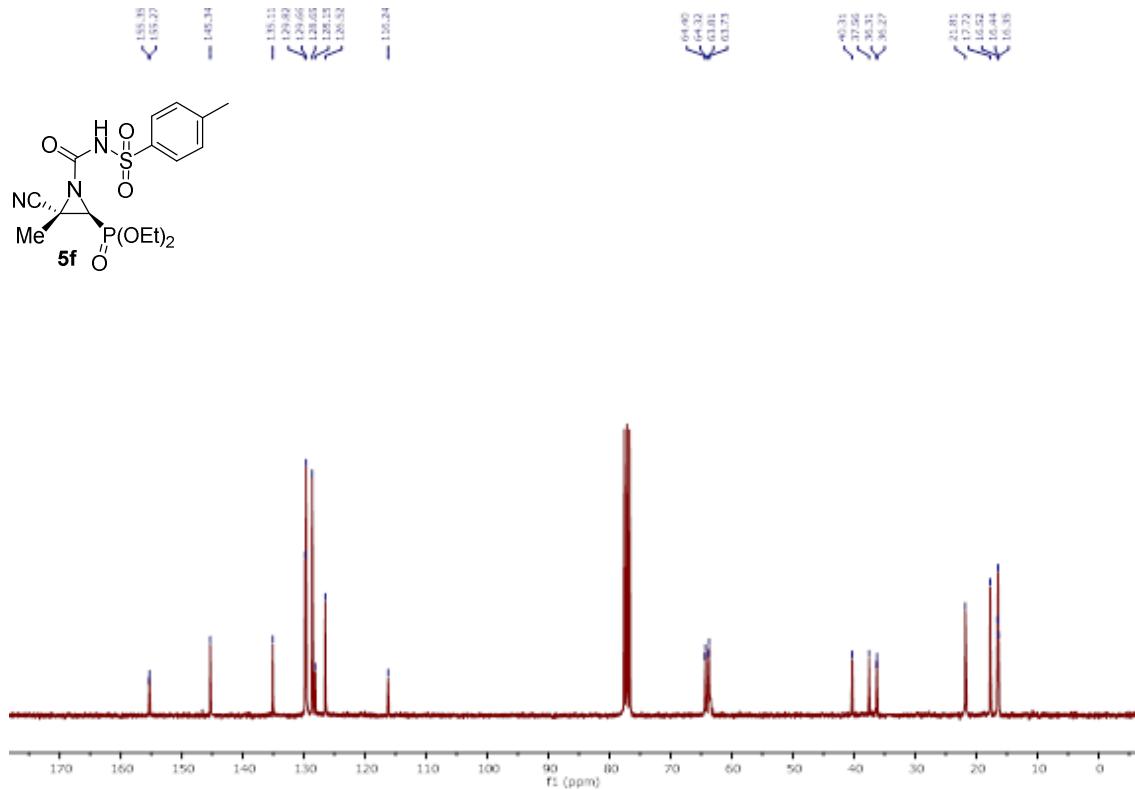
<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, MeOD) of compound 5e.



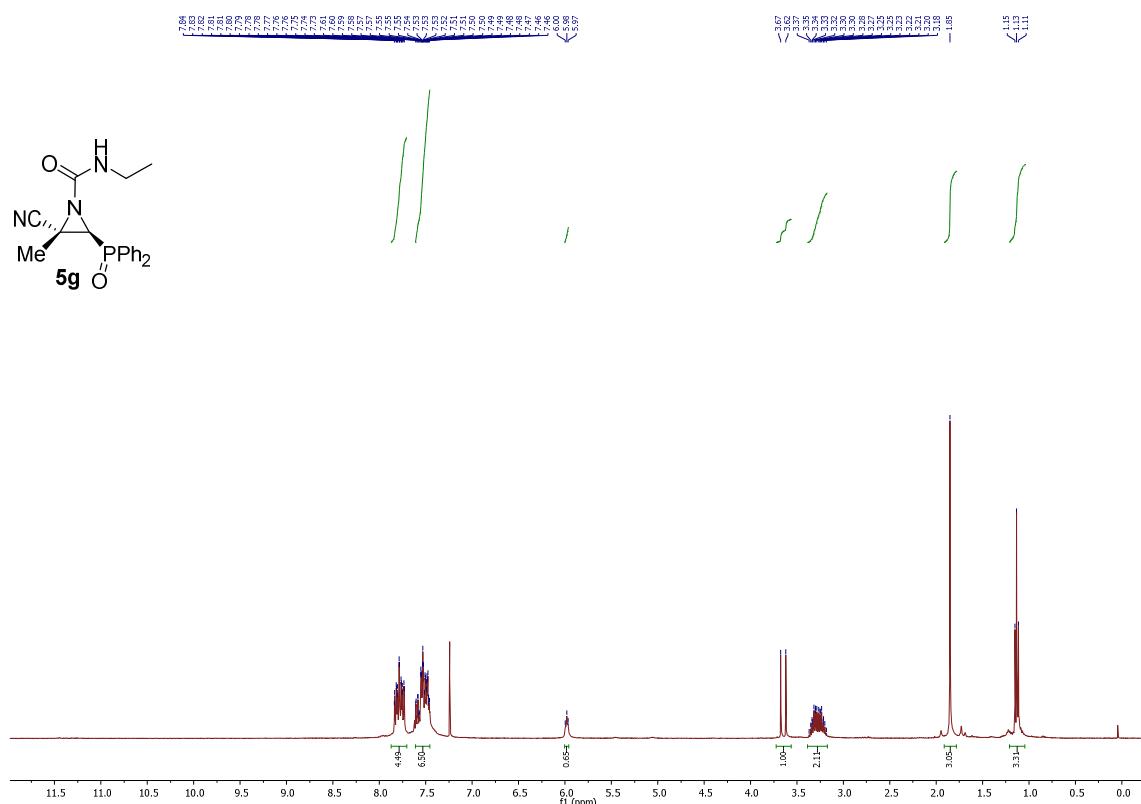
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 5f.



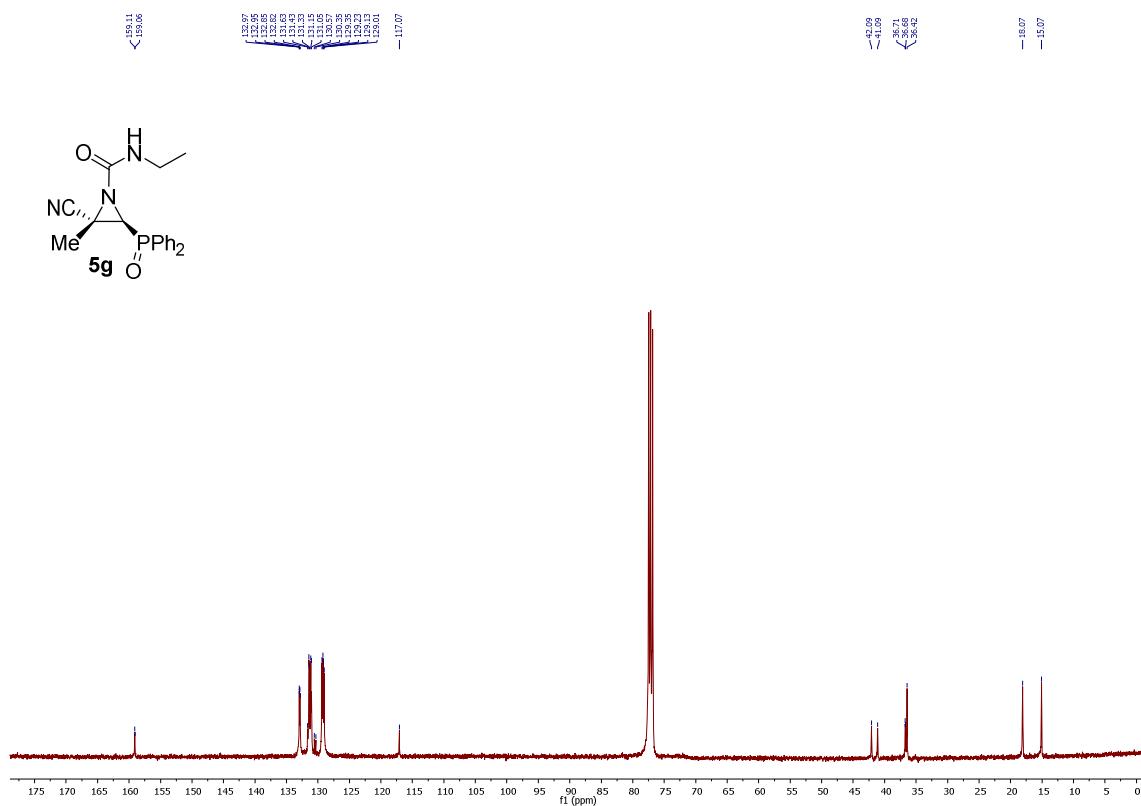
<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>) of compound 5f.



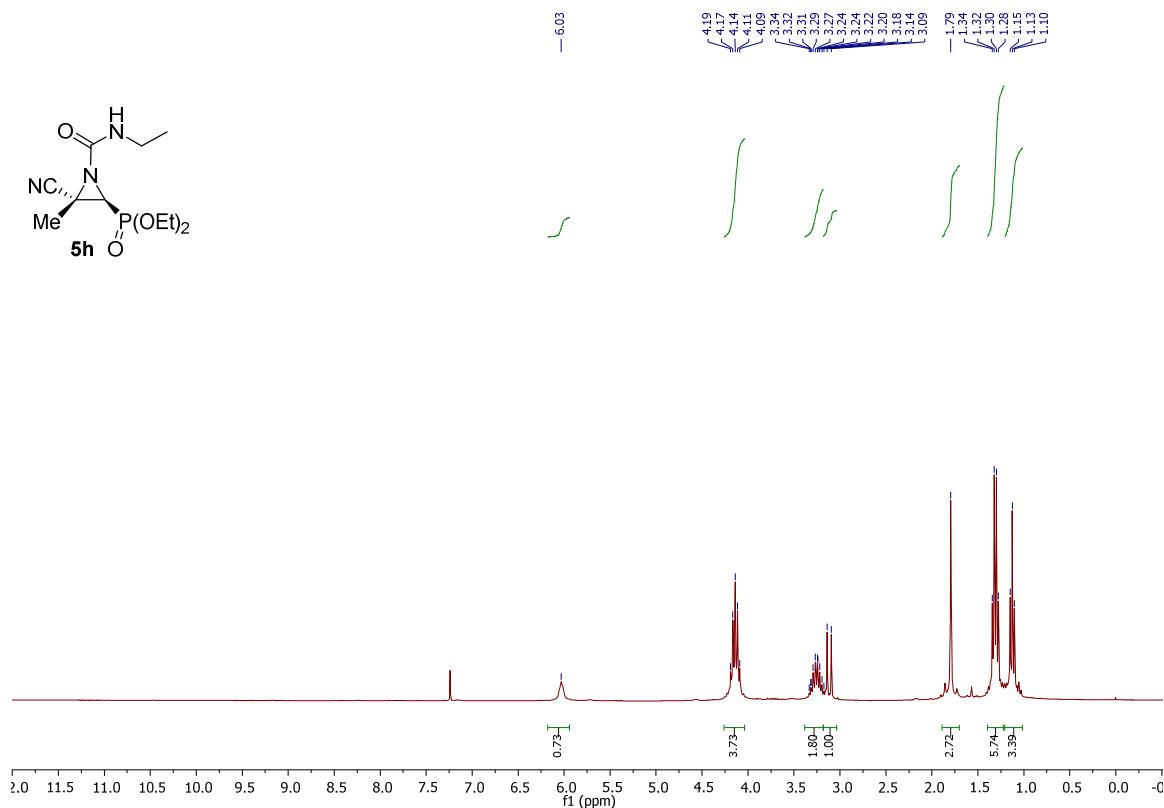
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound 5g.



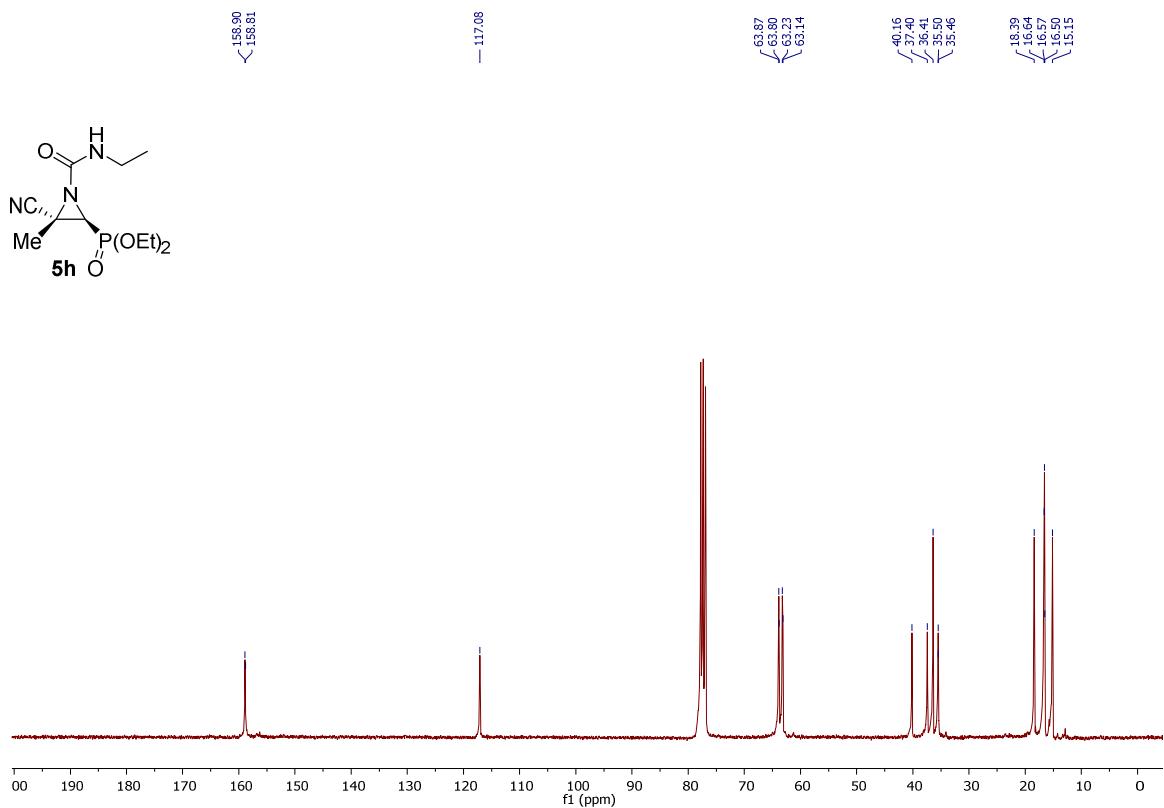
<sup>13</sup>C {<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>) of compound 5g.



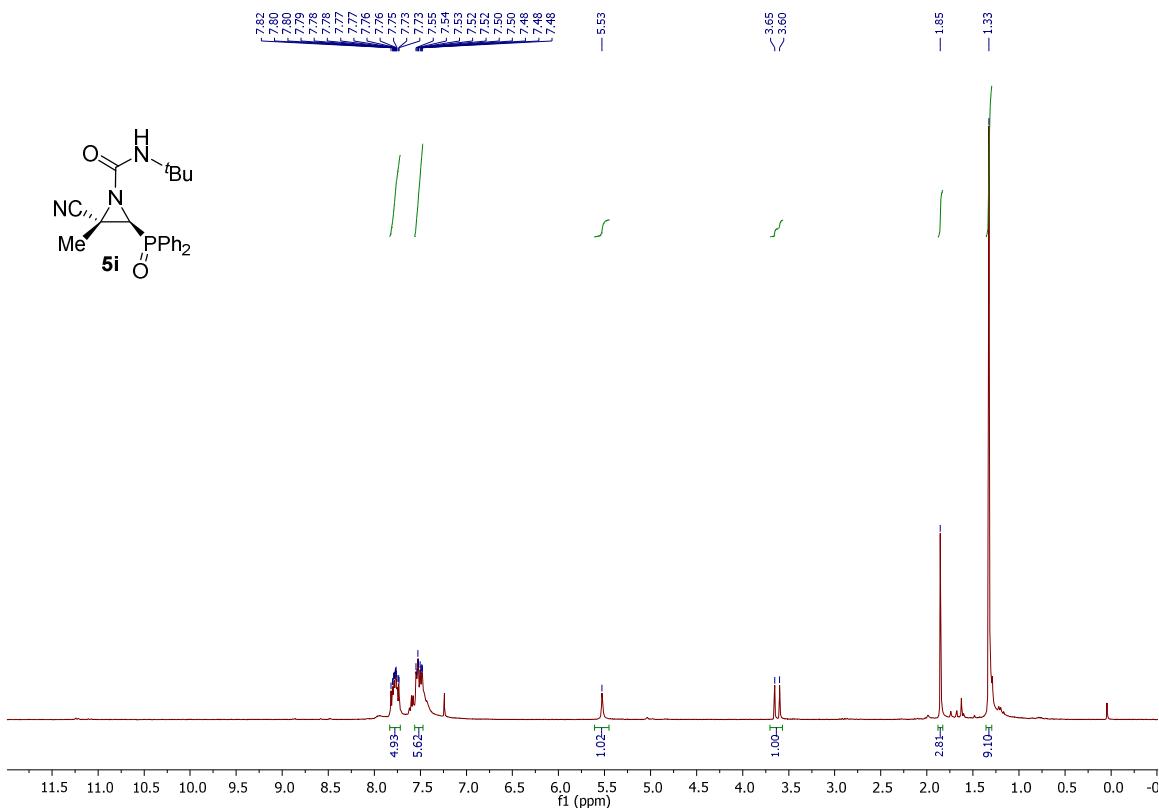
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound **5h**.



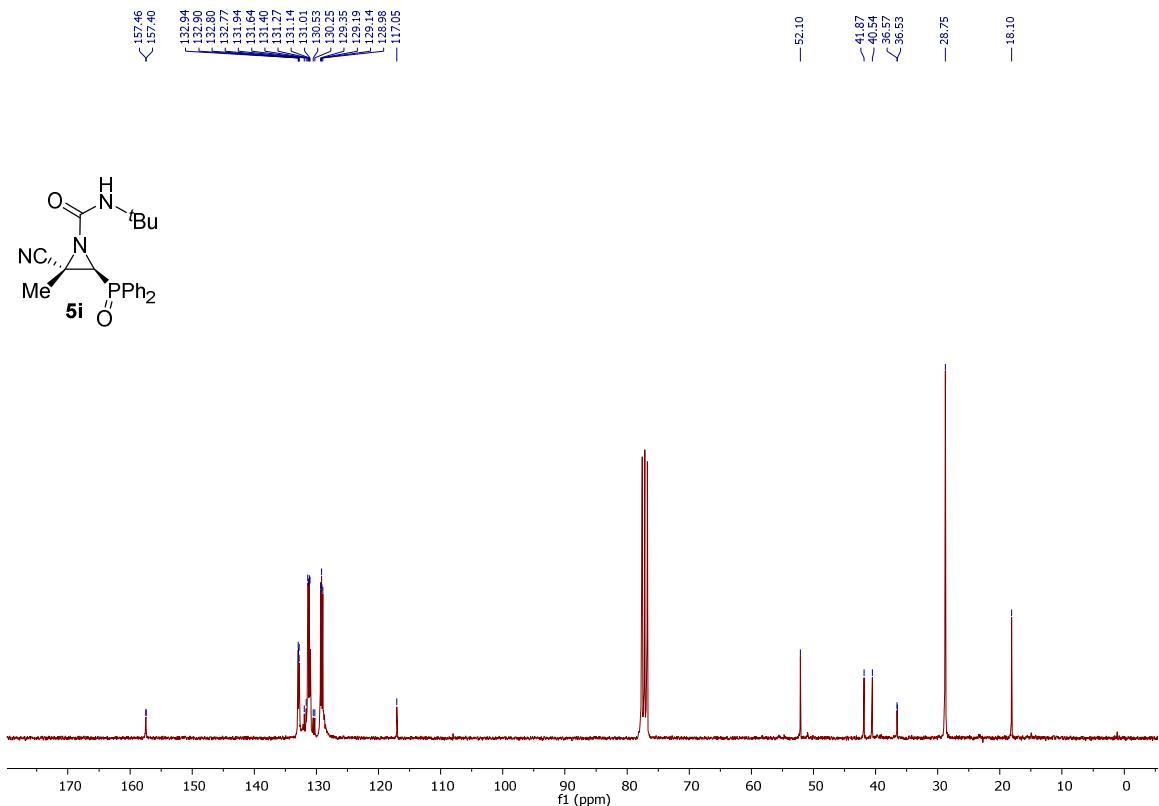
$^{13}\text{C}$  { $^1\text{H}$ } NMR (75 MHz,  $\text{CDCl}_3$ ) of compound **5h**.



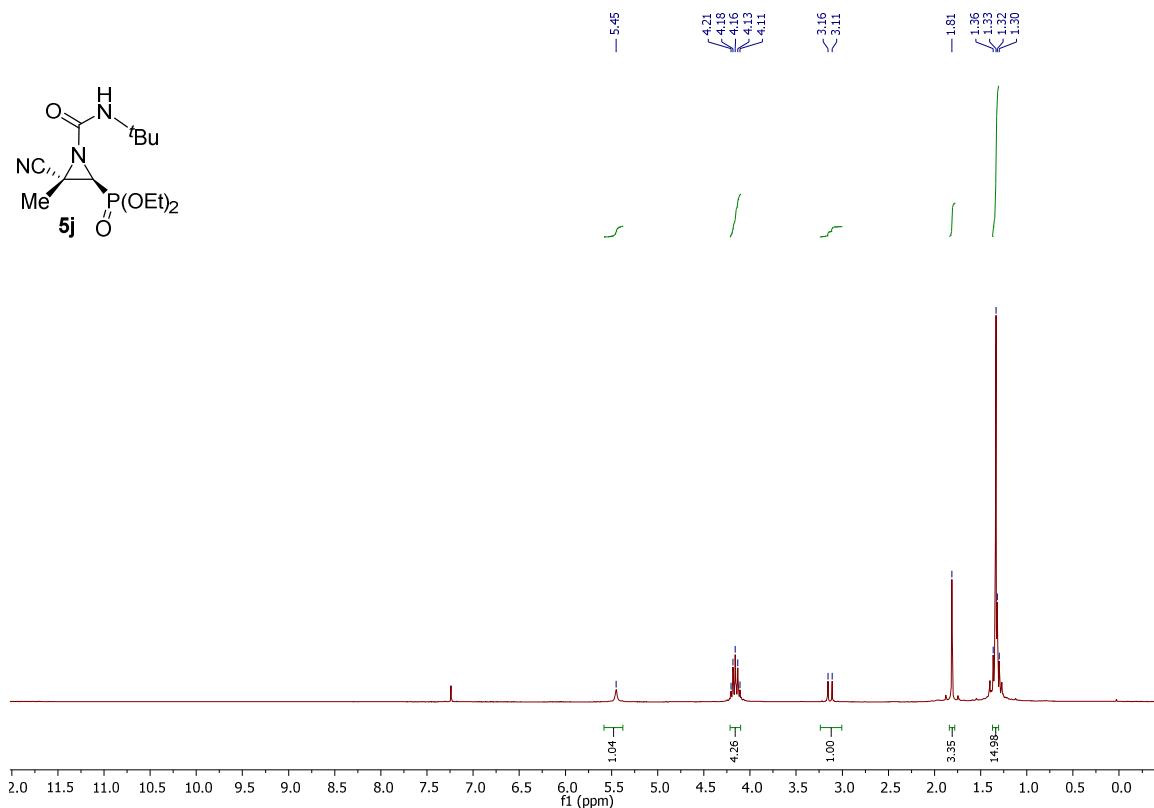
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **5i**.



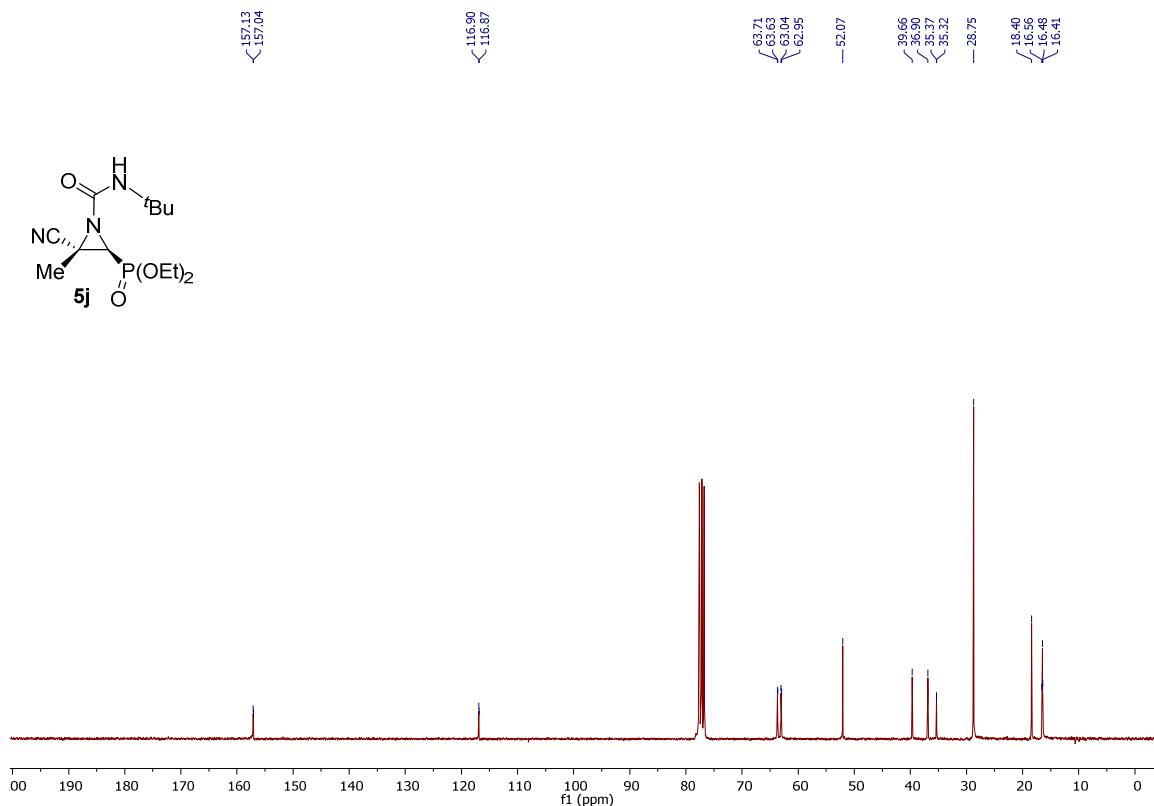
<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>) of compound **5i**.



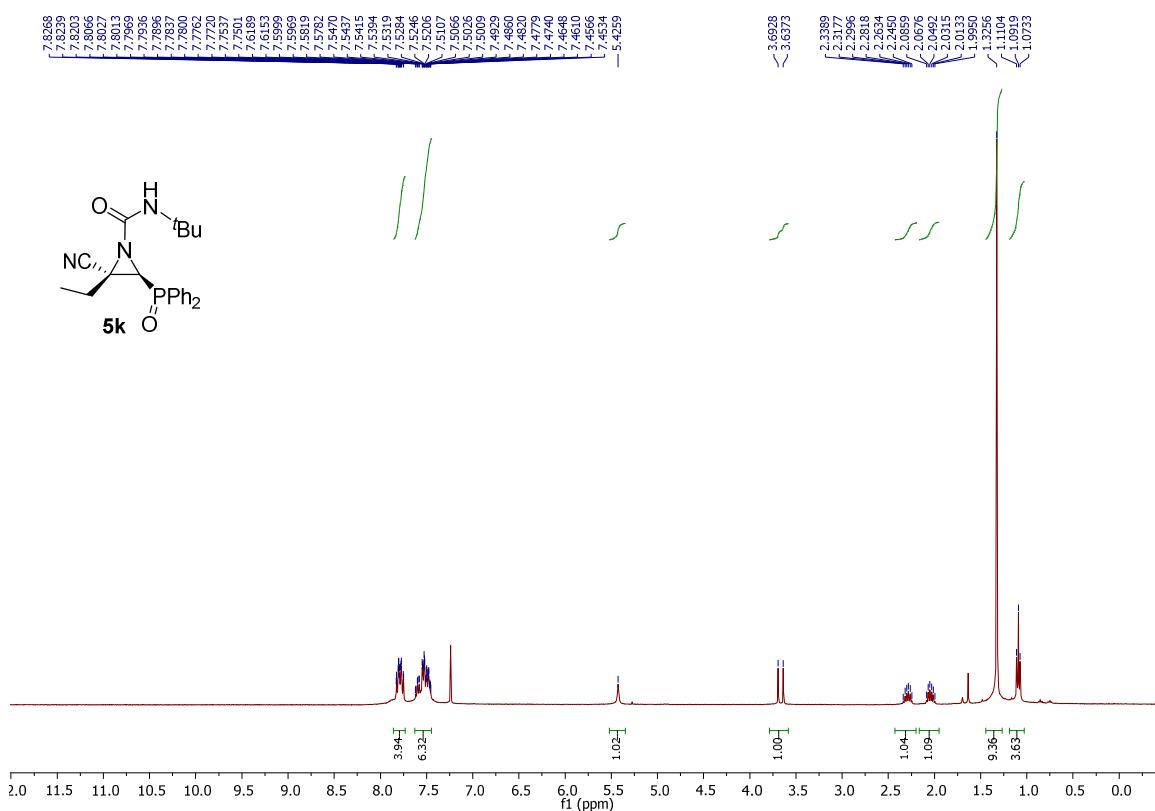
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 5j.



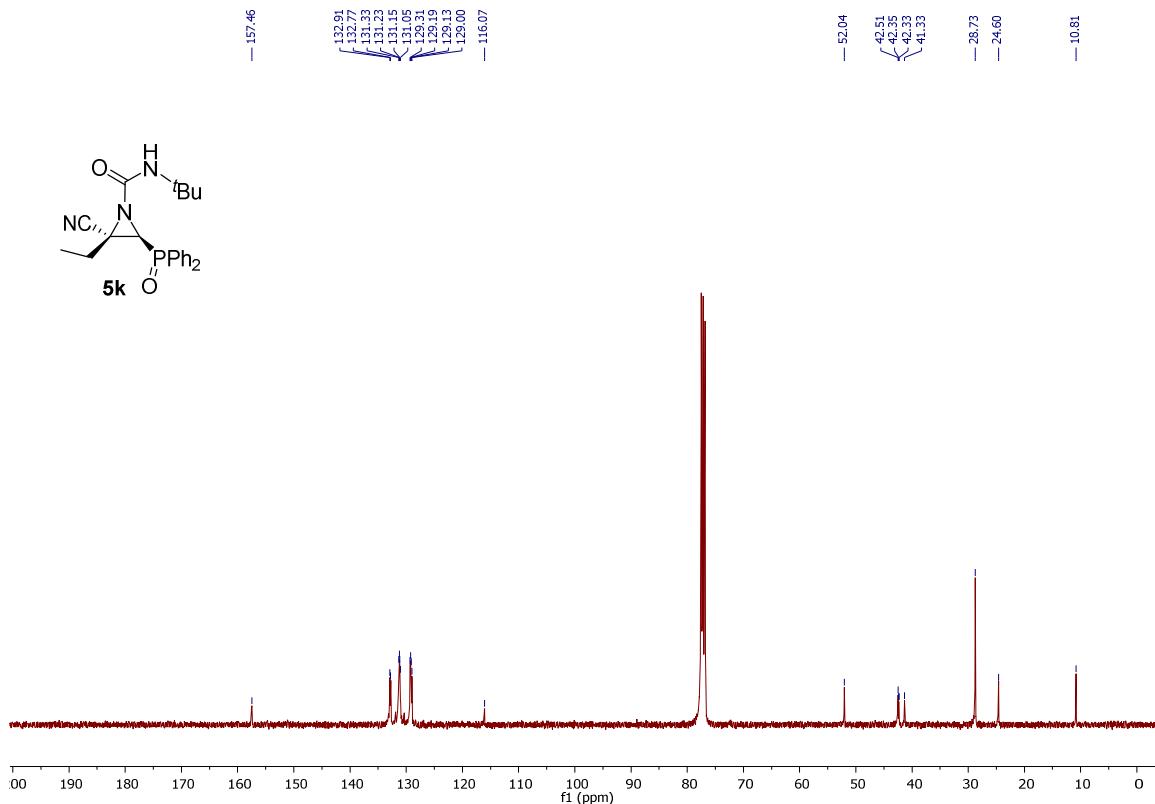
<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>) of compound 5j.



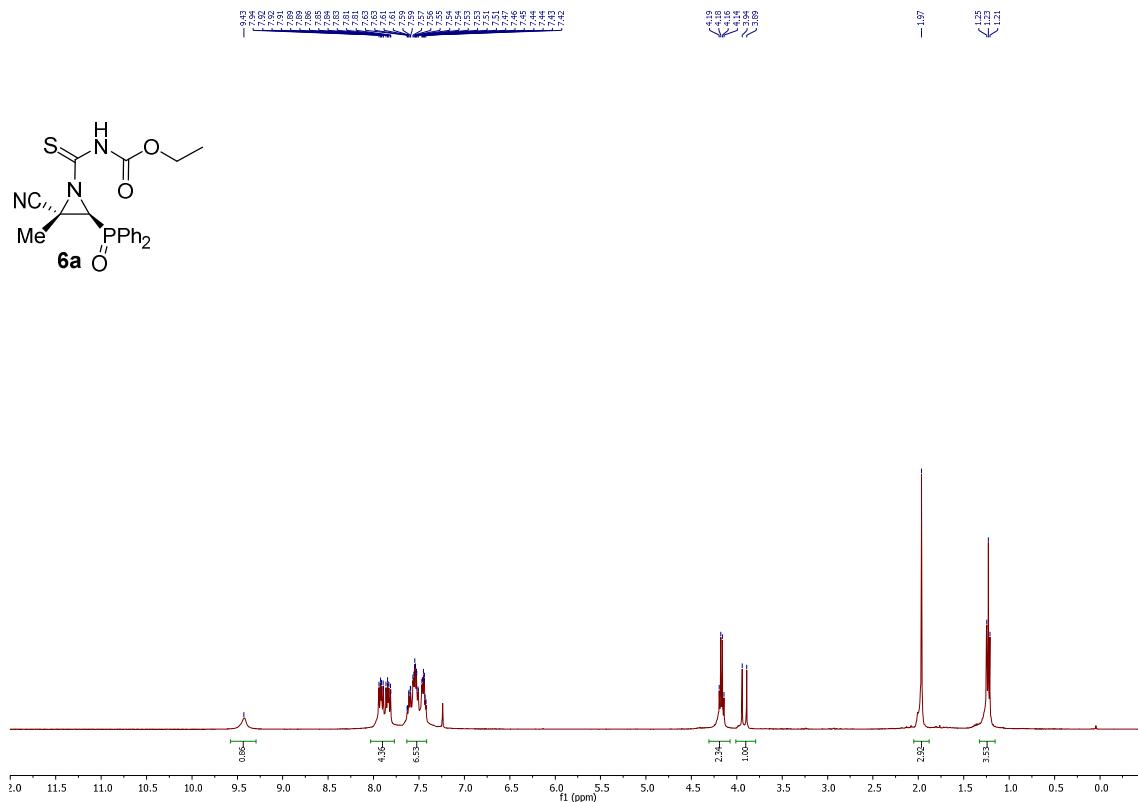
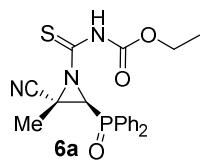
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **5k**.



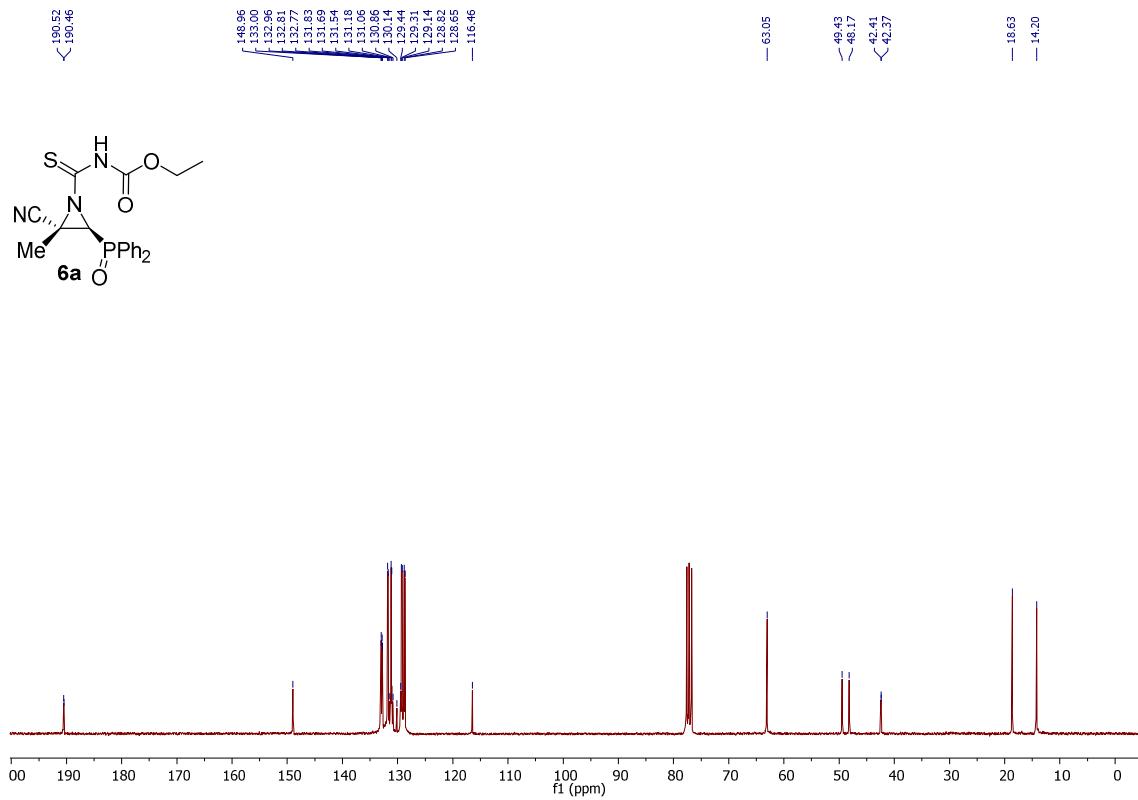
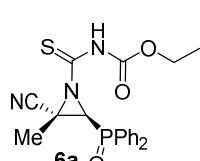
$^{13}\text{C}$  { $^1\text{H}$ } NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **5k**.



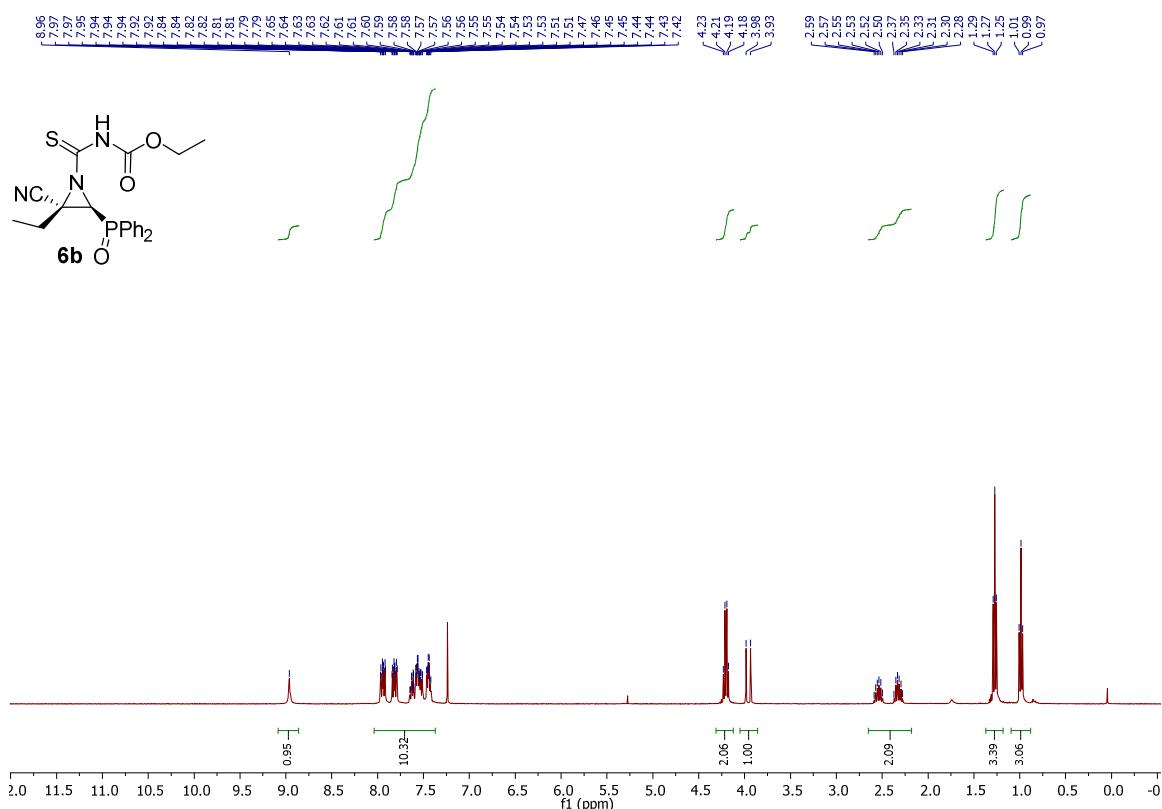
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **6a**.



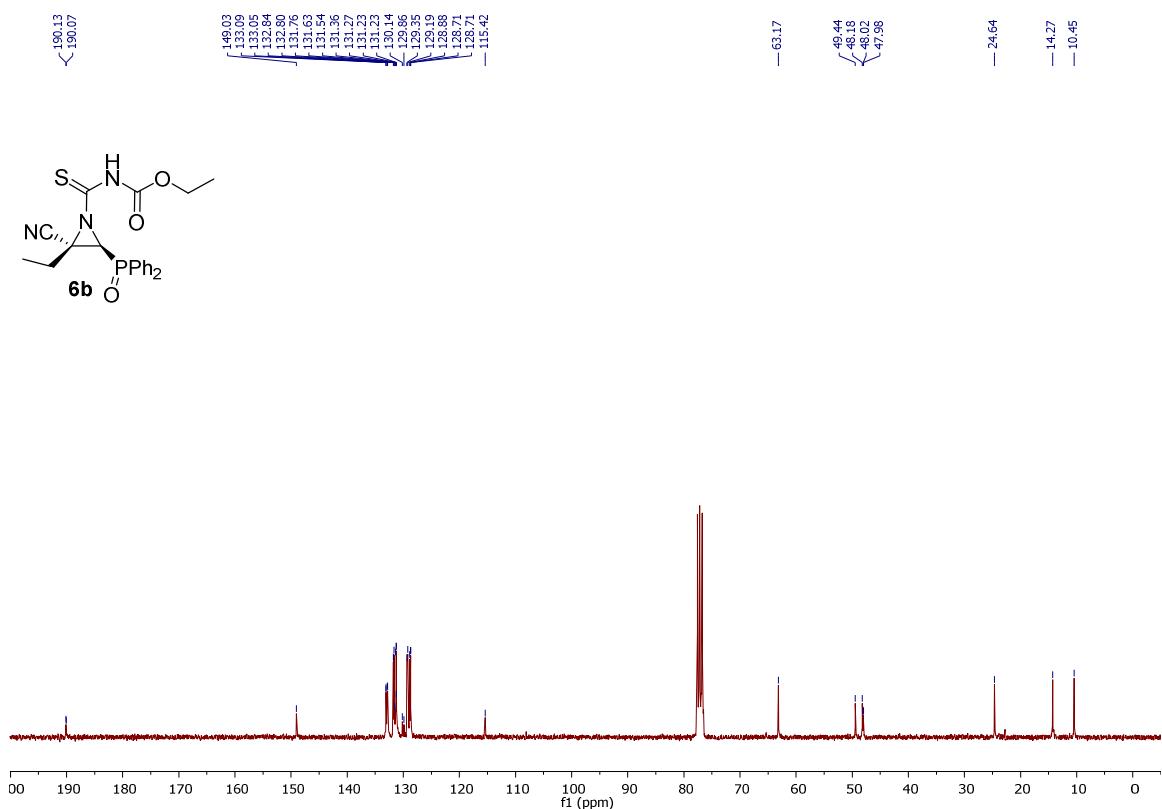
$^{13}\text{C}$  { $^1\text{H}$ } NMR (75 MHz,  $\text{CDCl}_3$ ) of compound **6a**.



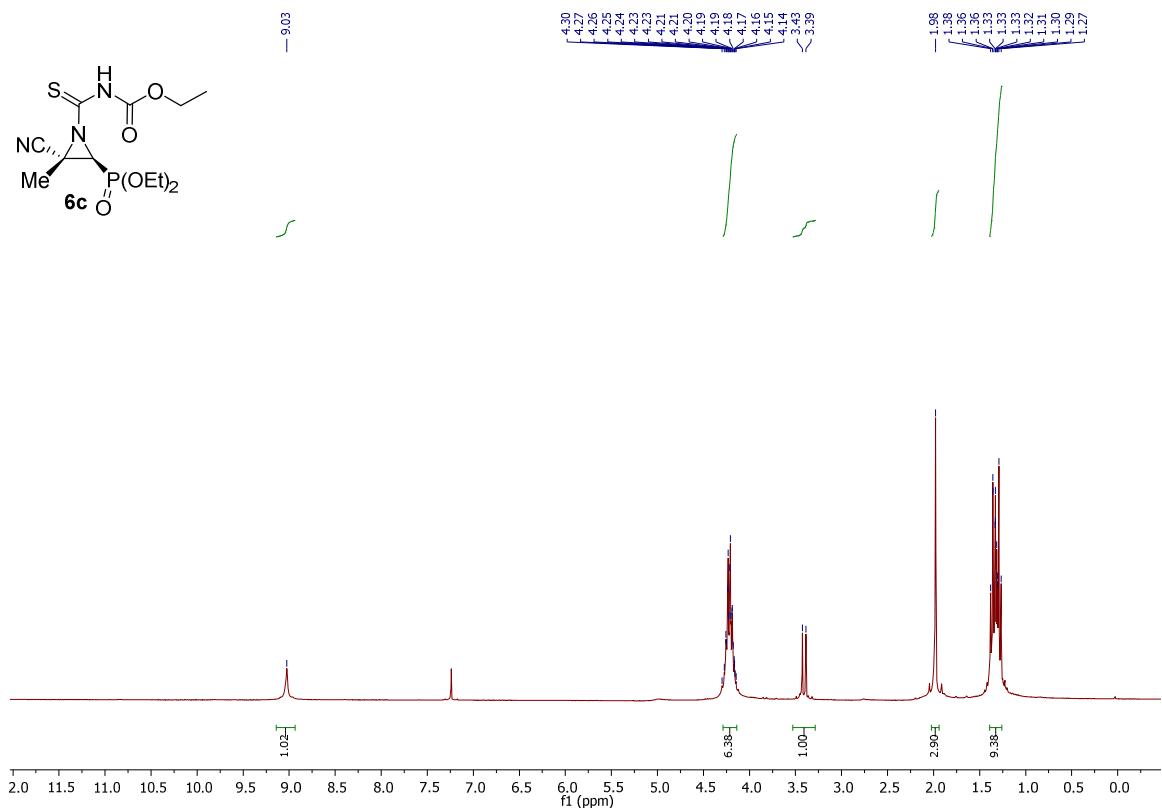
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **6b**.



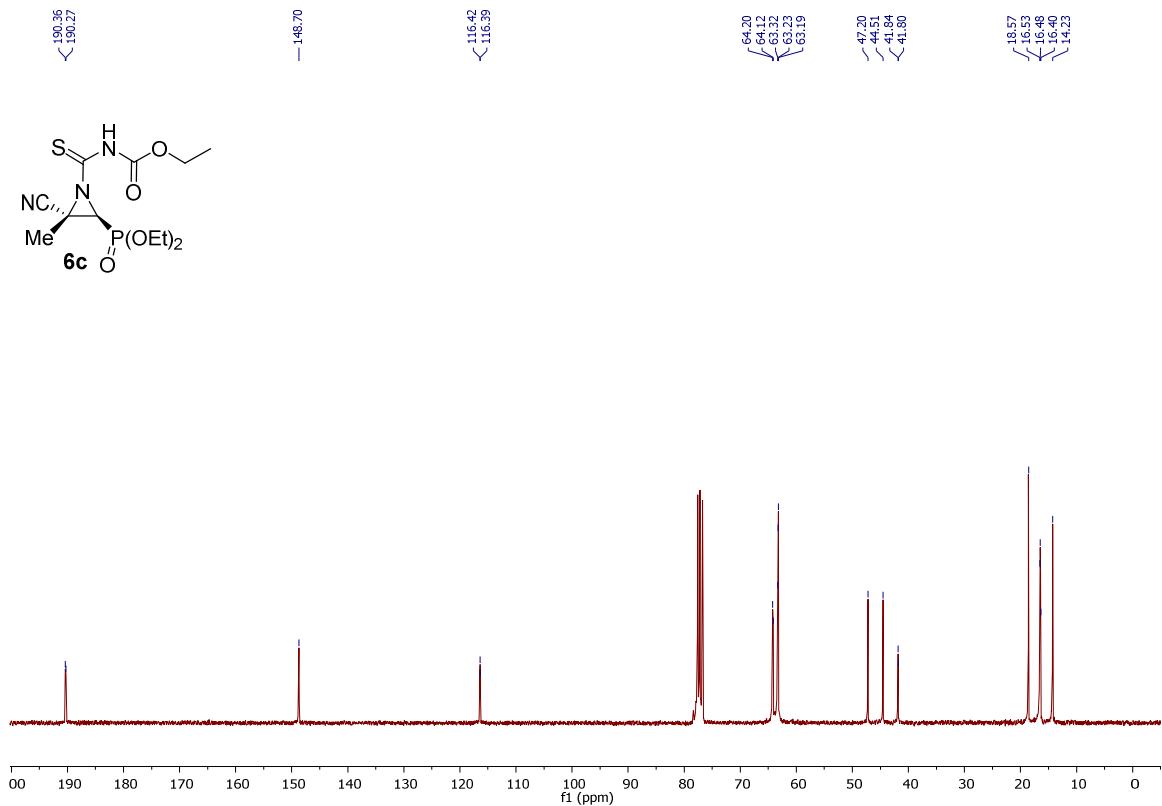
$^{13}\text{C}$  { $^1\text{H}$ } NMR (75 MHz,  $\text{CDCl}_3$ ) of compound **6b**.



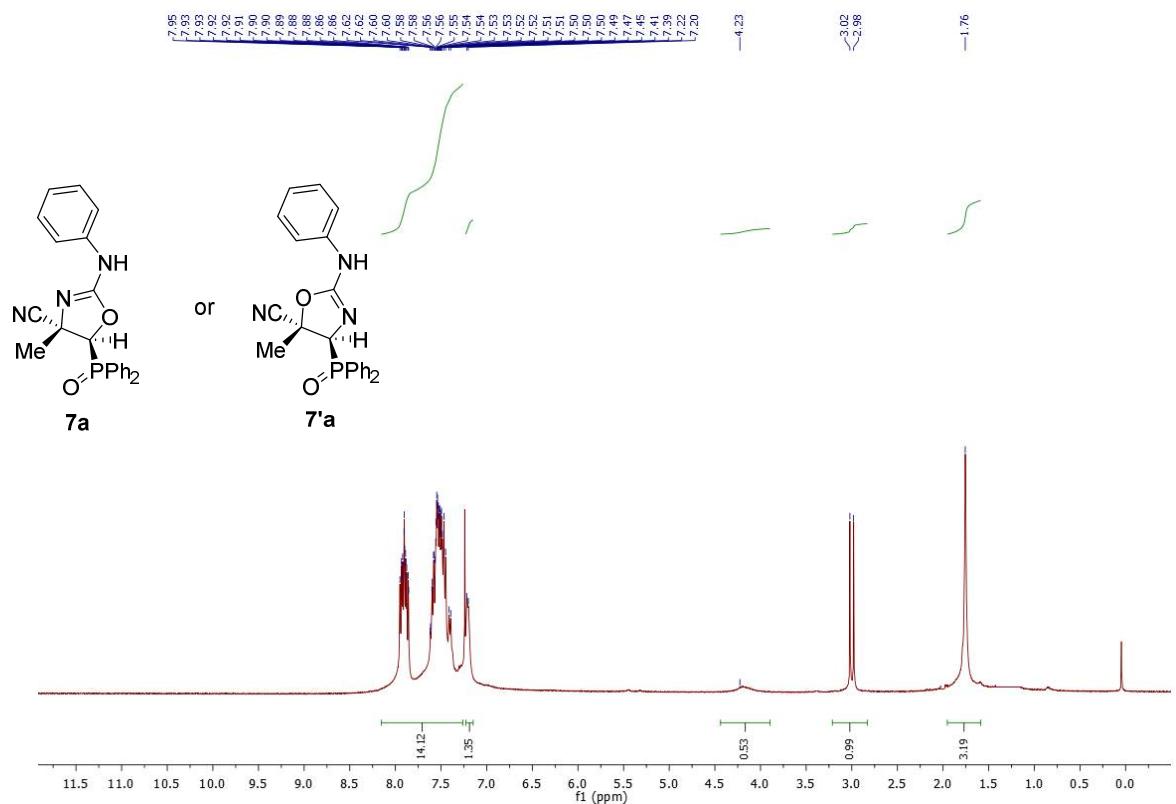
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 6c.



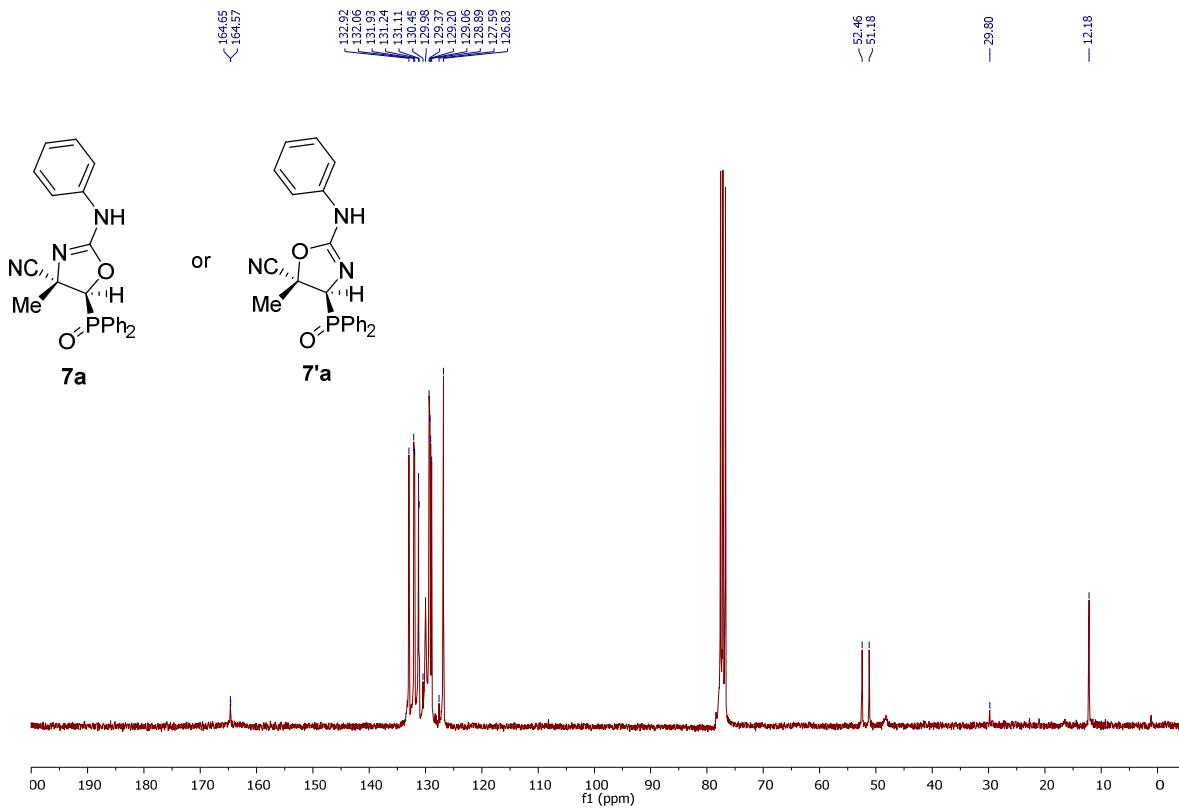
<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>) of compound 6c.



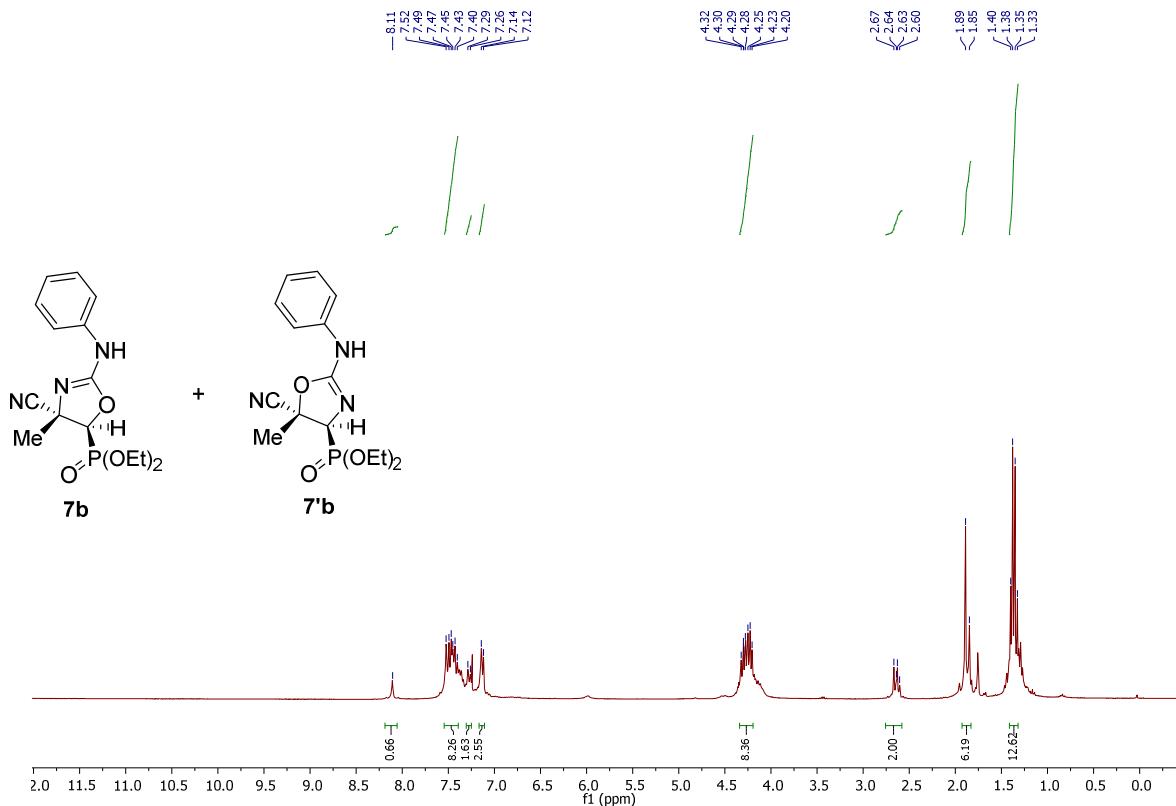
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound 7a or 7'a.



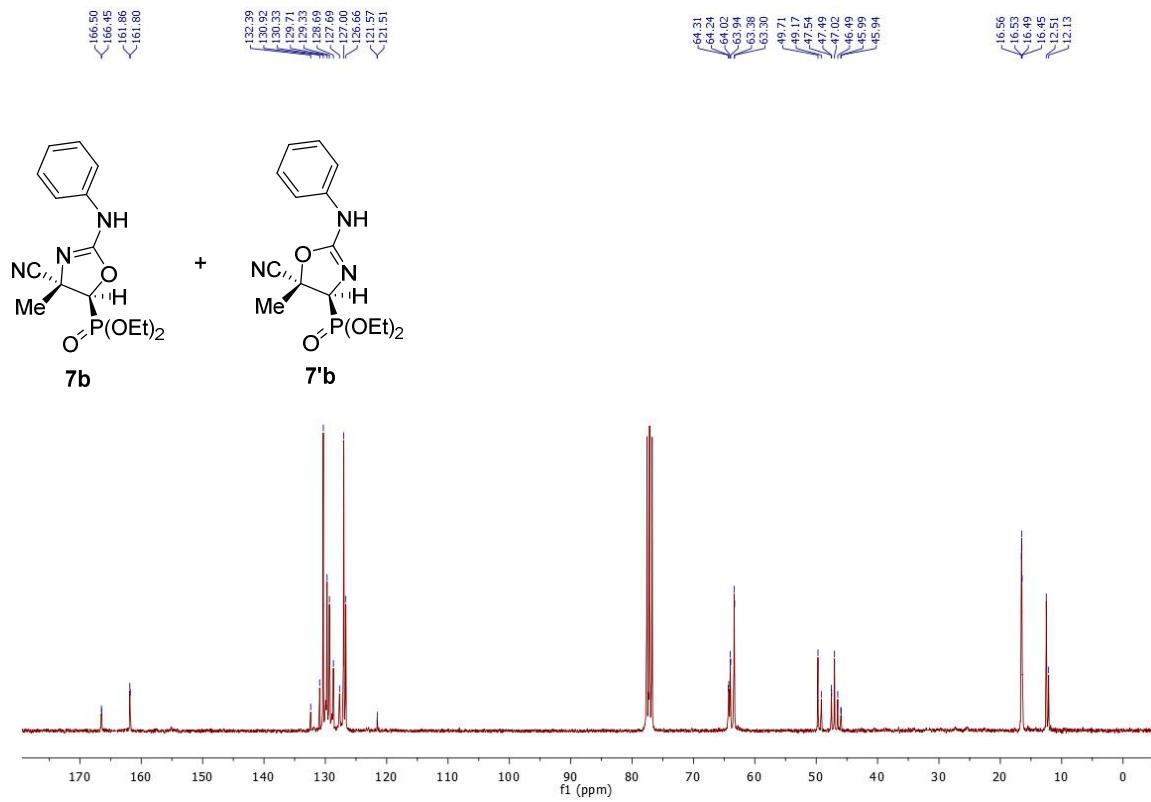
<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>) of compound 7a or 7'a.



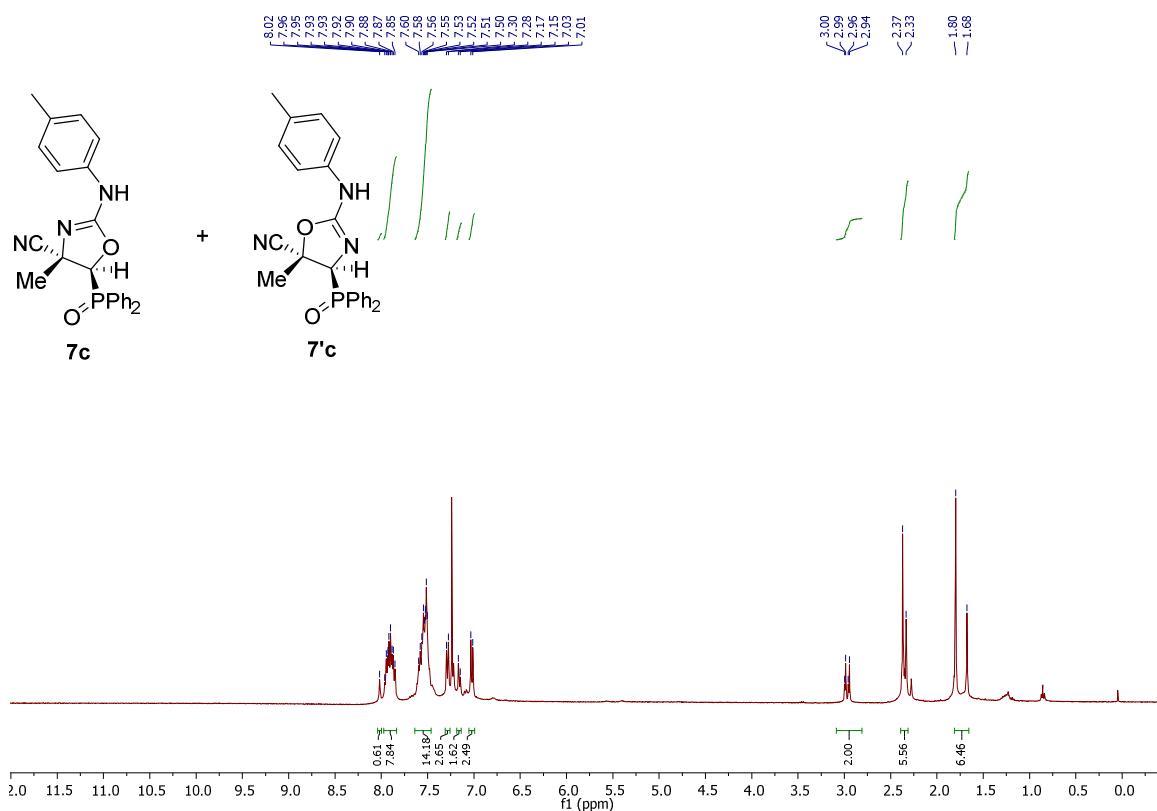
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 7b + 7'b.



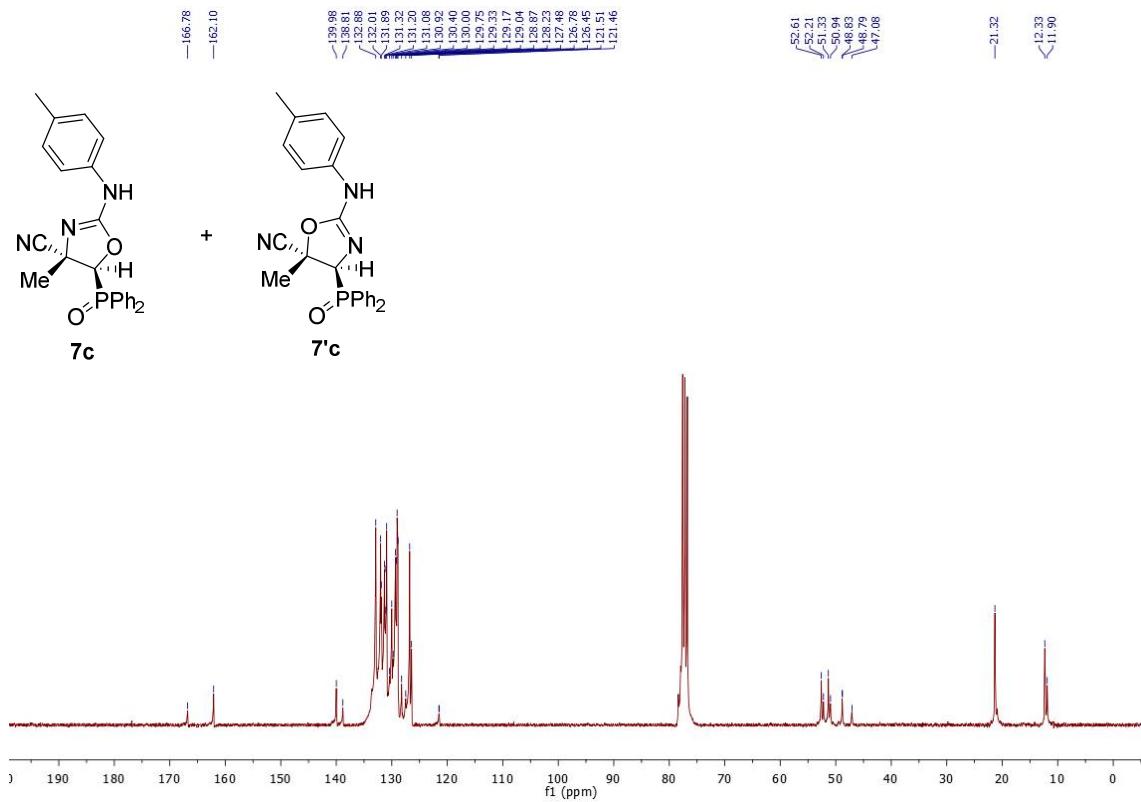
<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>) of compound 7b + 7'b.



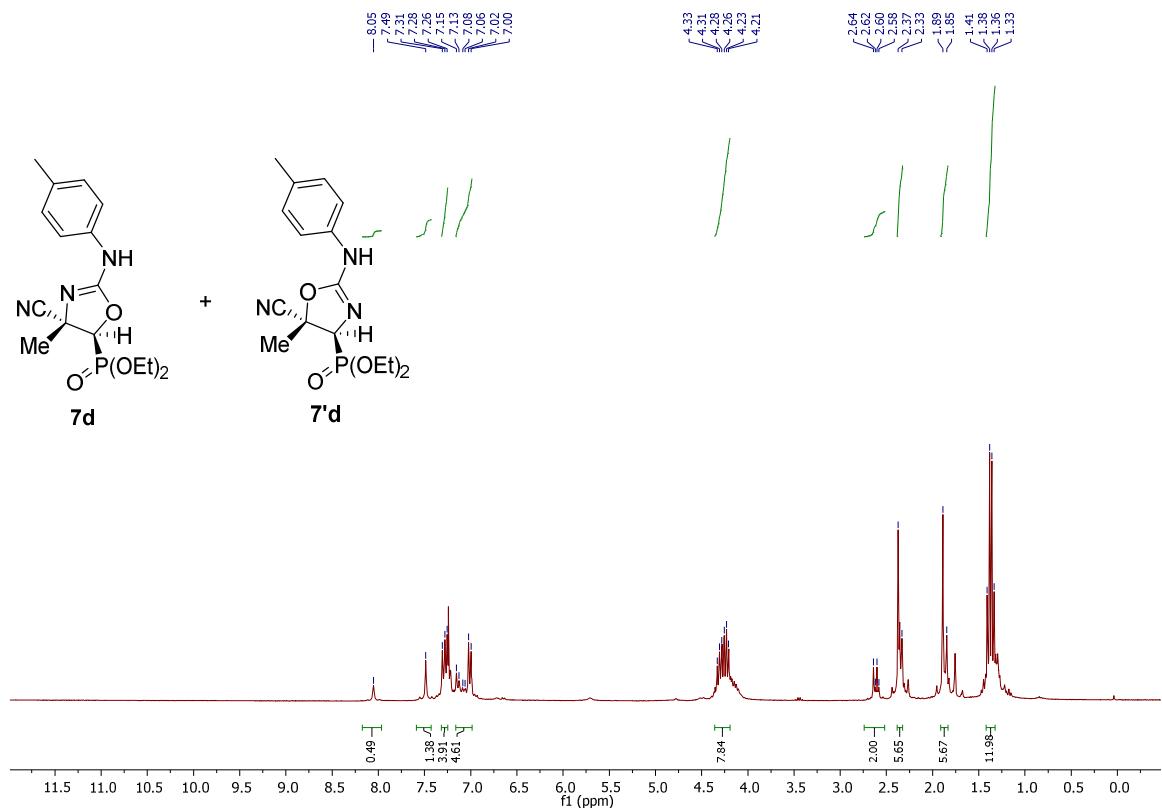
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound 7c + 7'c.



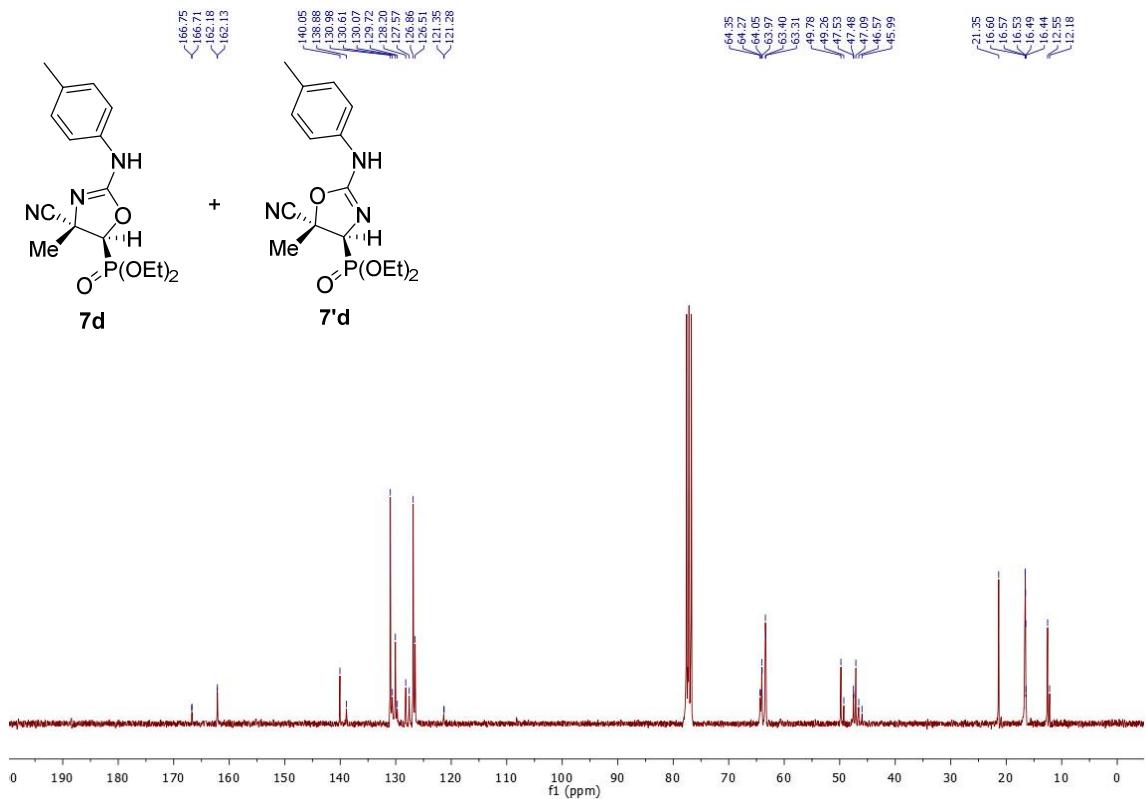
<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>) of compound **7c + 7'c**.



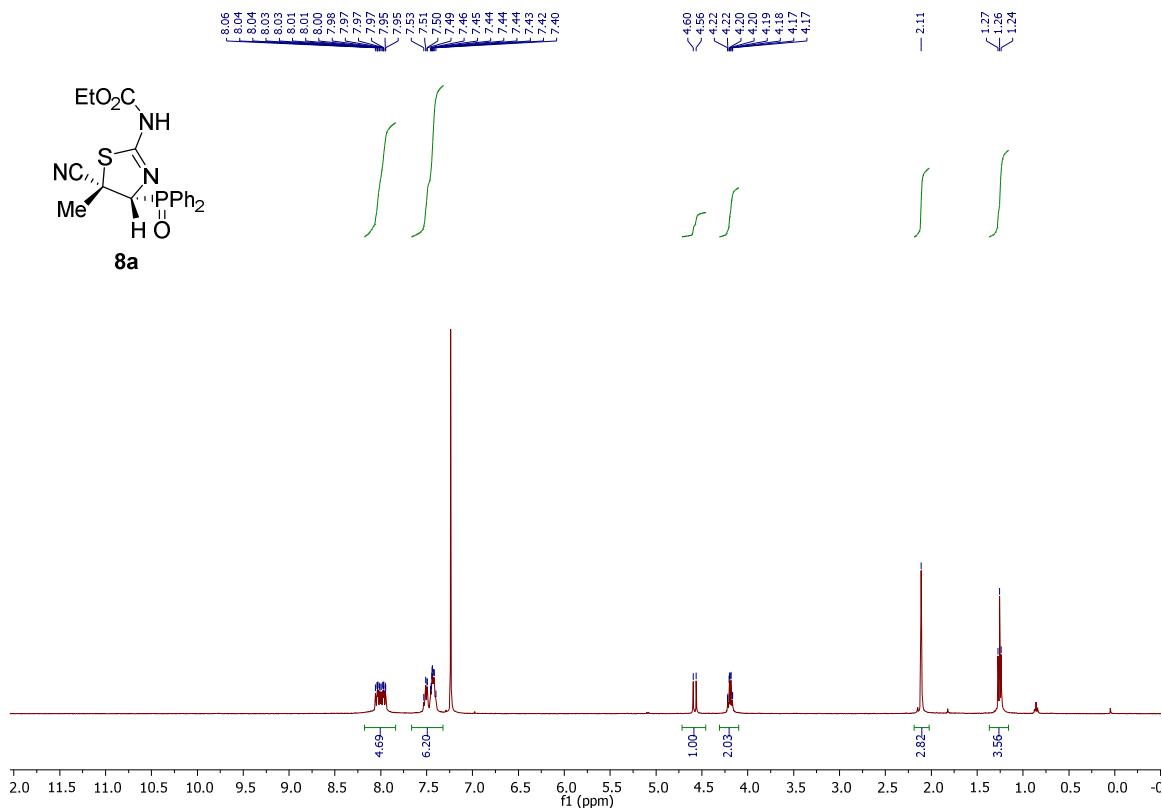
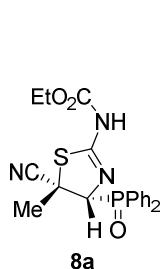
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 7d + 7'd.



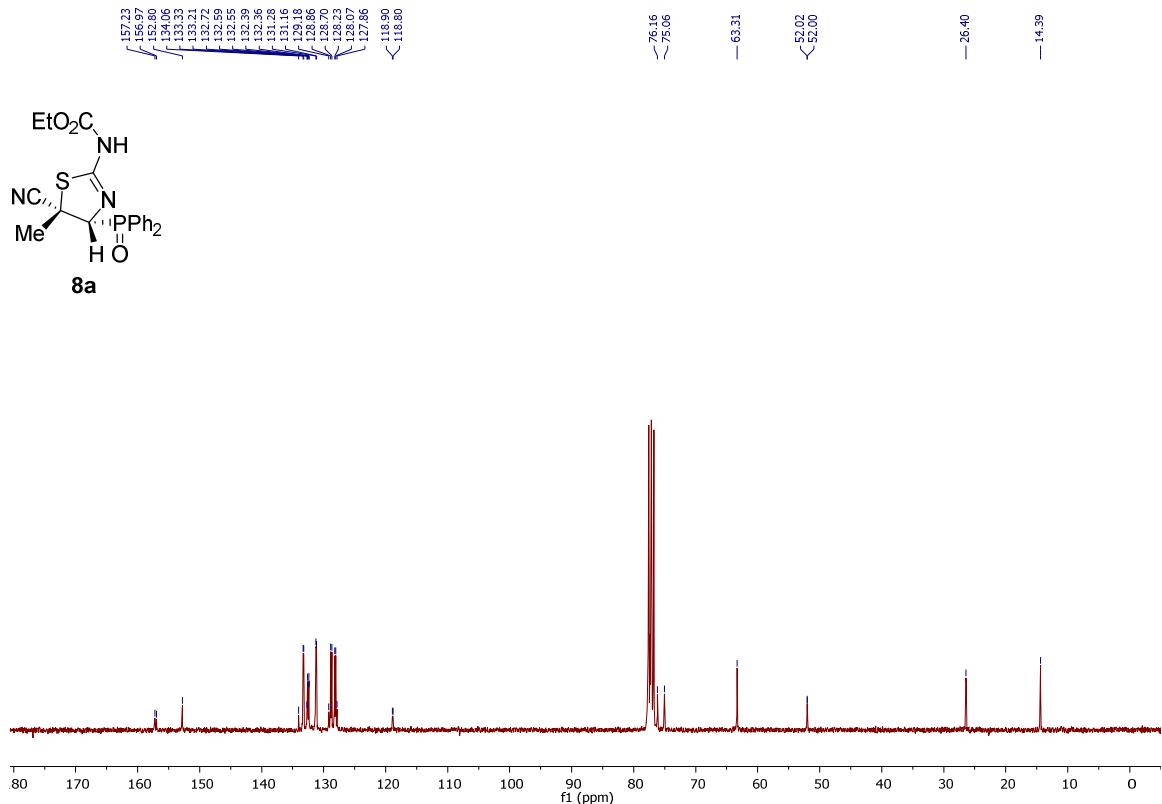
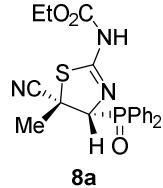
<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>) of compound 7d + 7'd.



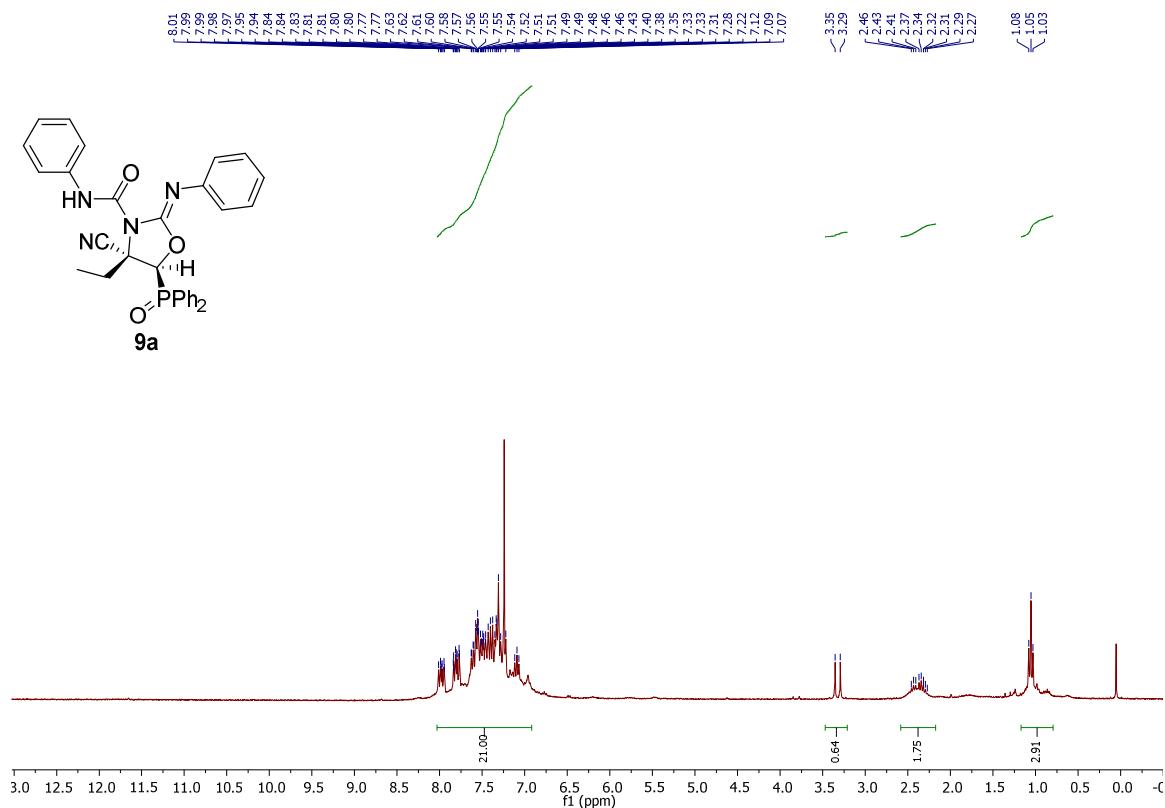
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound 8a.



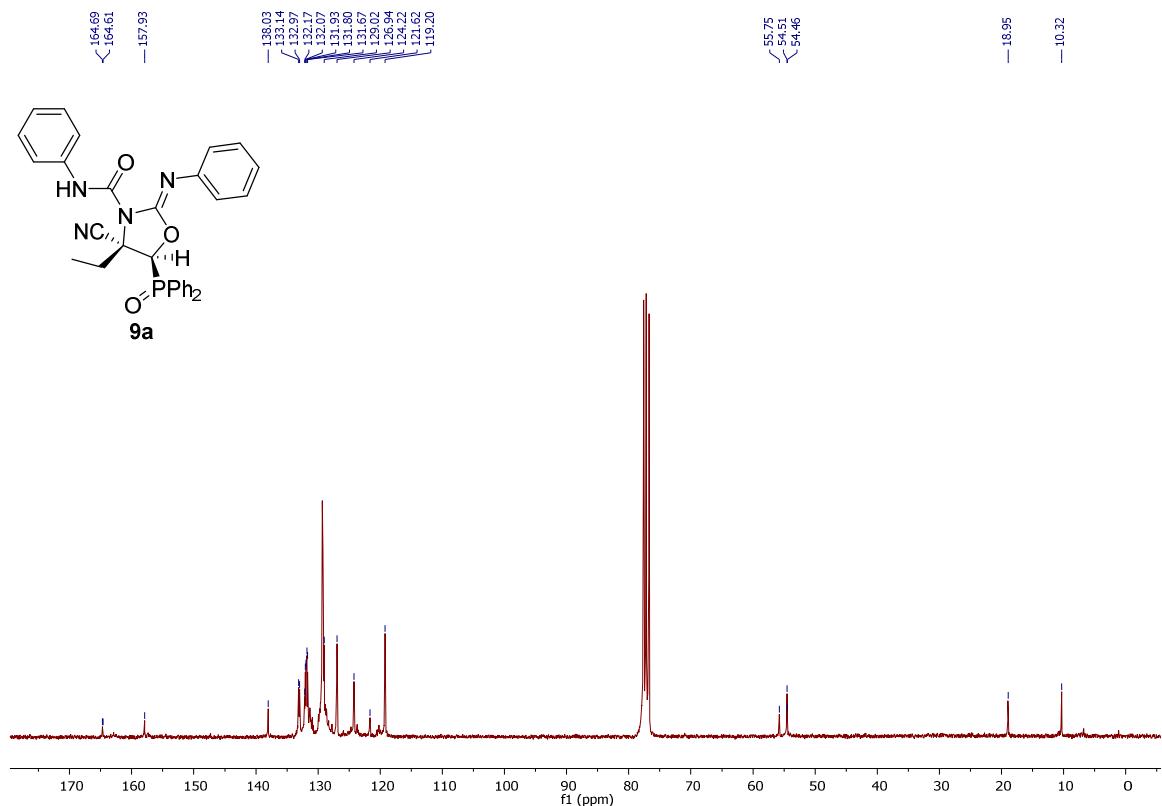
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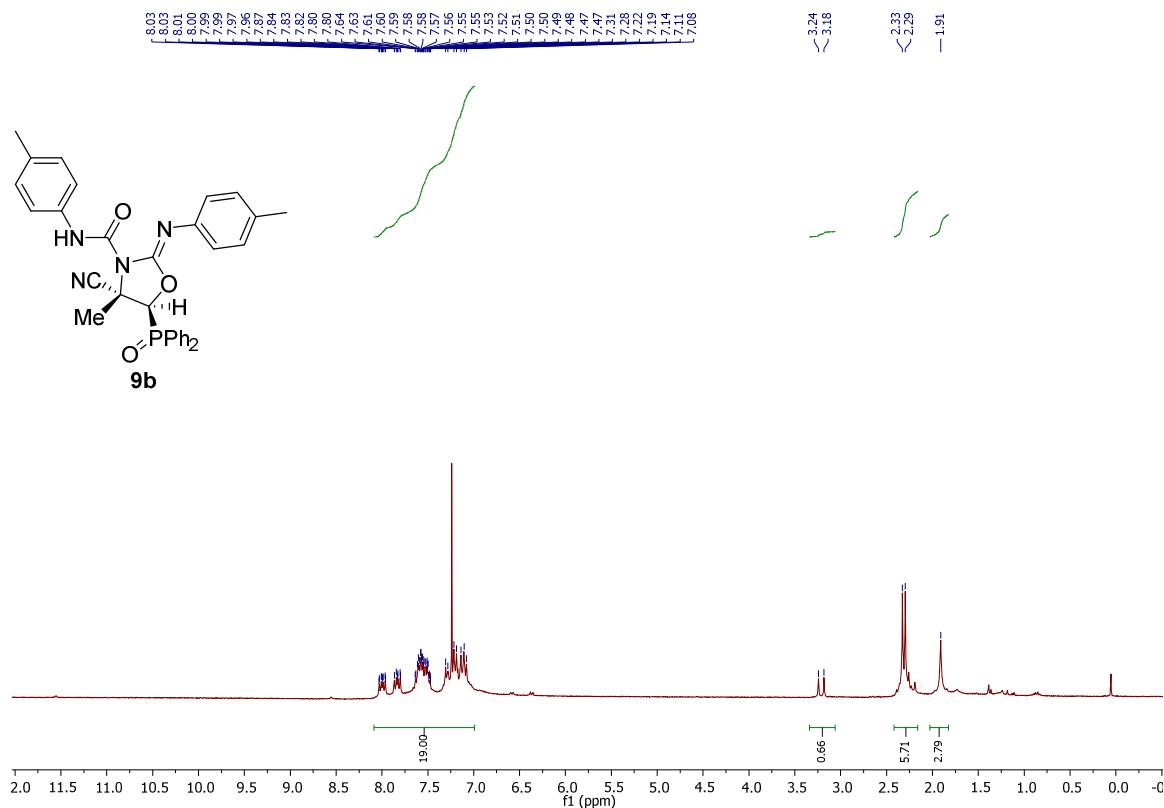
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) of compound **9a**.



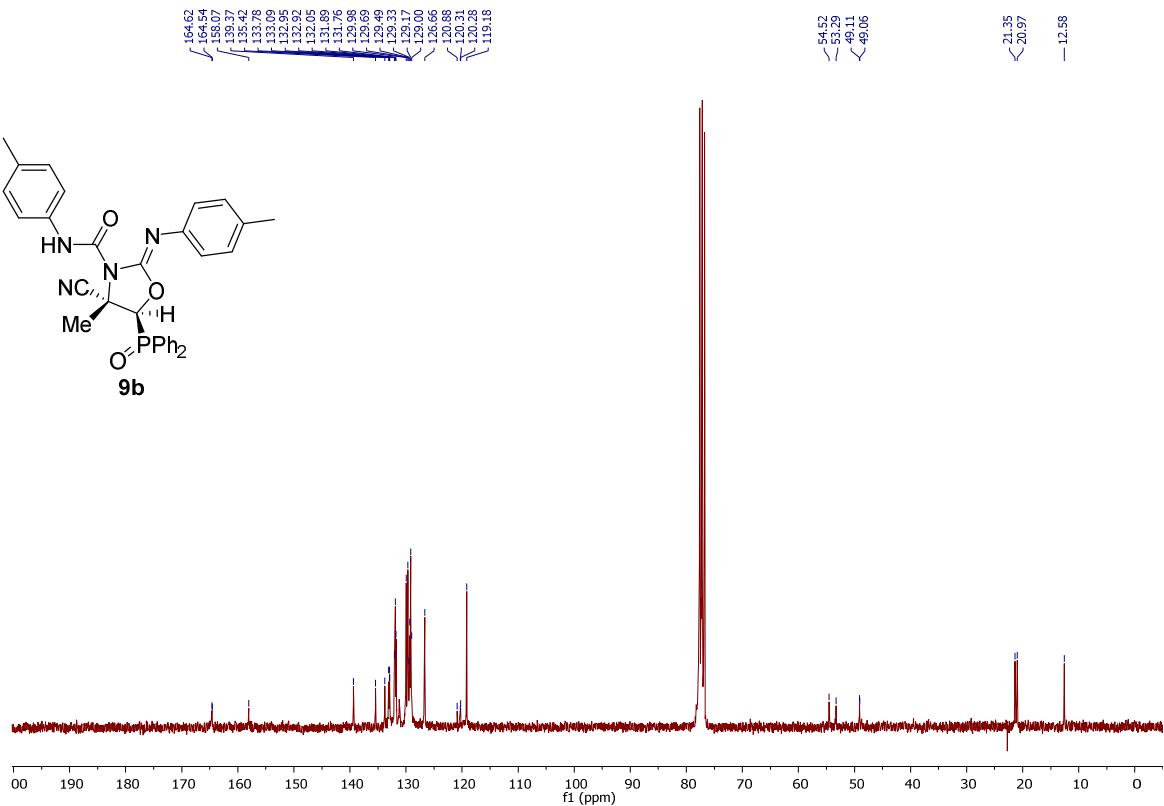
$^{13}\text{C}$  { $^1\text{H}$ } NMR (75 MHz,  $\text{CDCl}_3$ ) of compound **9a**.



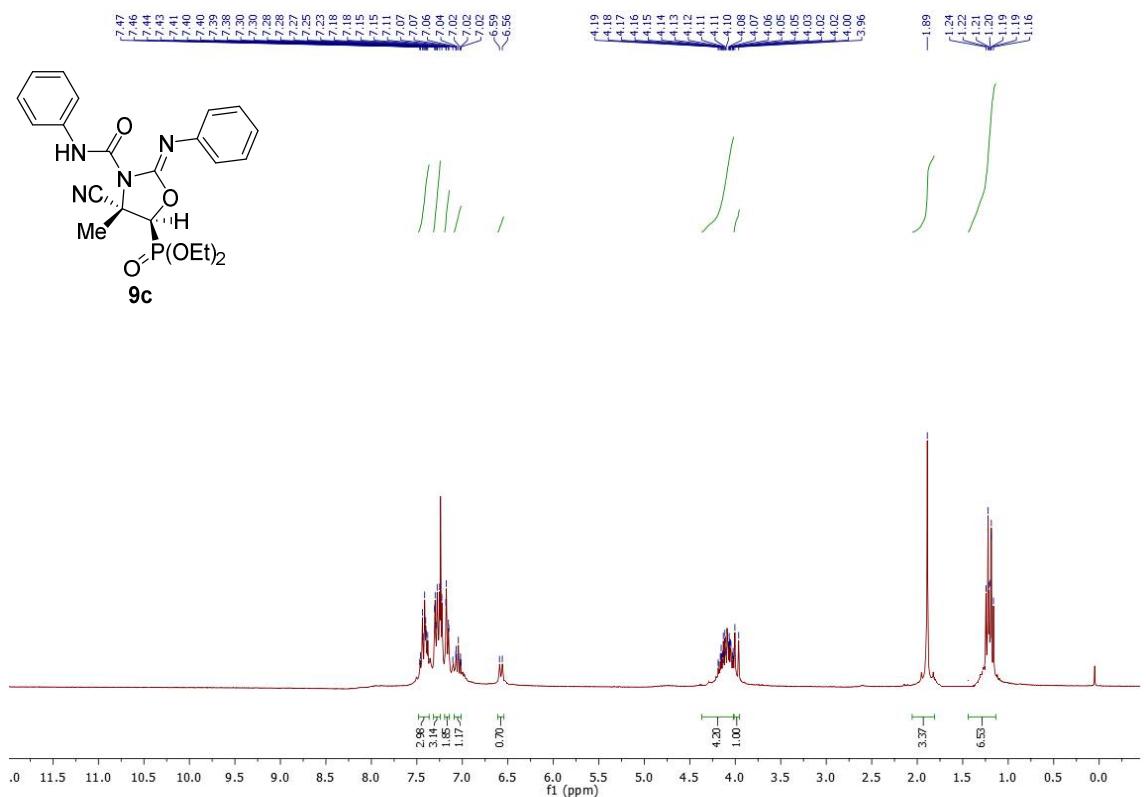
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound **9b**.



<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>) of compound **9b**.



<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 9c.



<sup>13</sup>C {<sup>1</sup>H} NMR (75 MHz, CDCl<sub>3</sub>) of compound 9c.

