

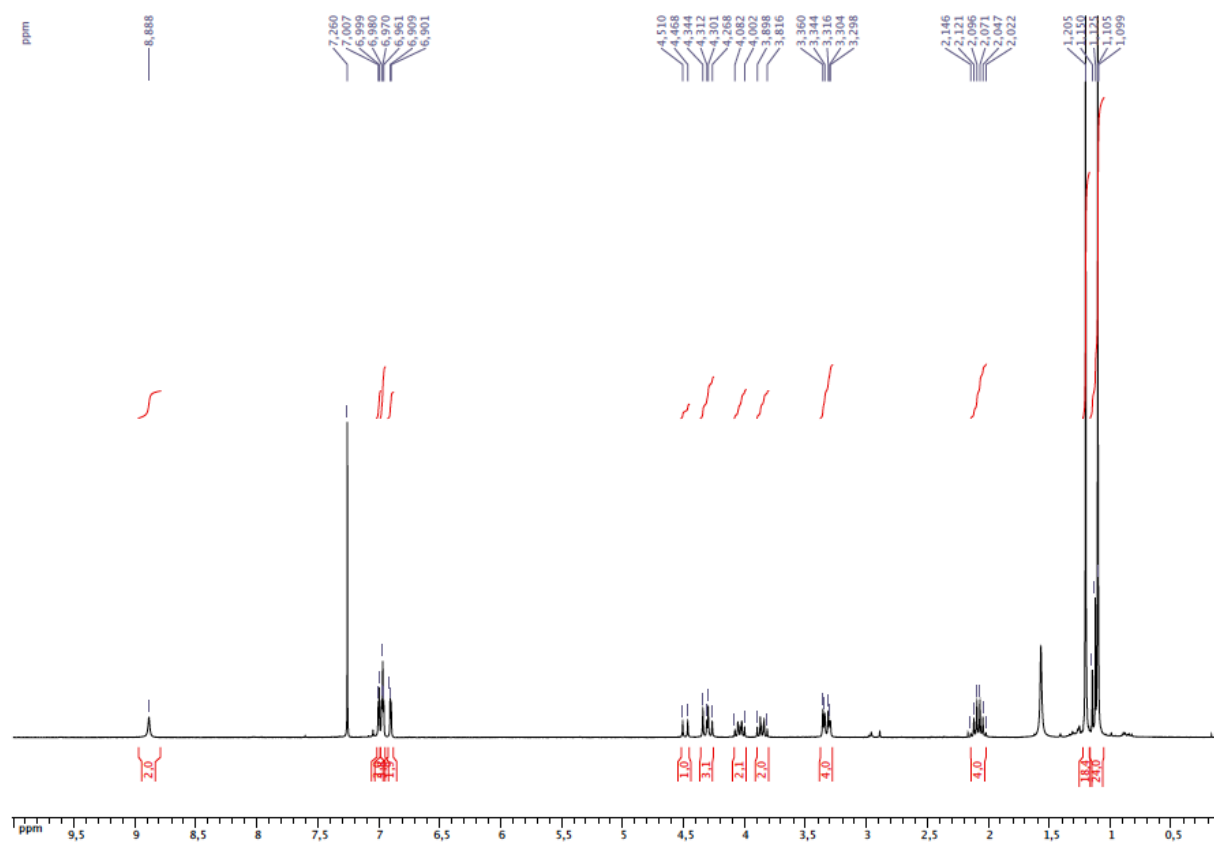
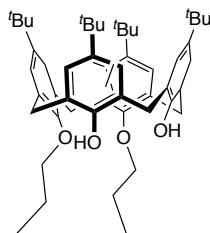
# How do positions of phosphito units on a calix[4]arene platform affect the enantioselectivity of a catalytic reaction?

Shaima Hkiri, David Sémeril

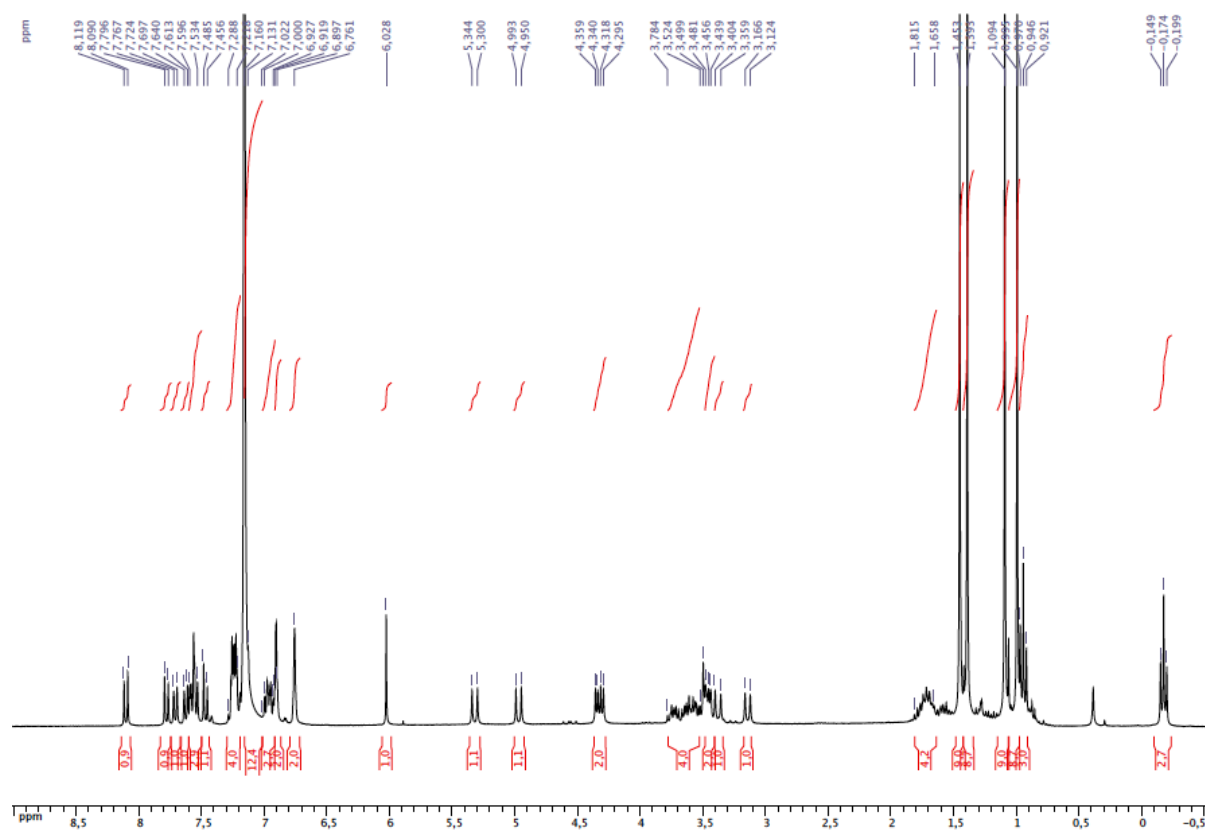
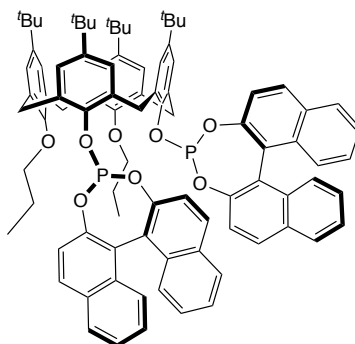
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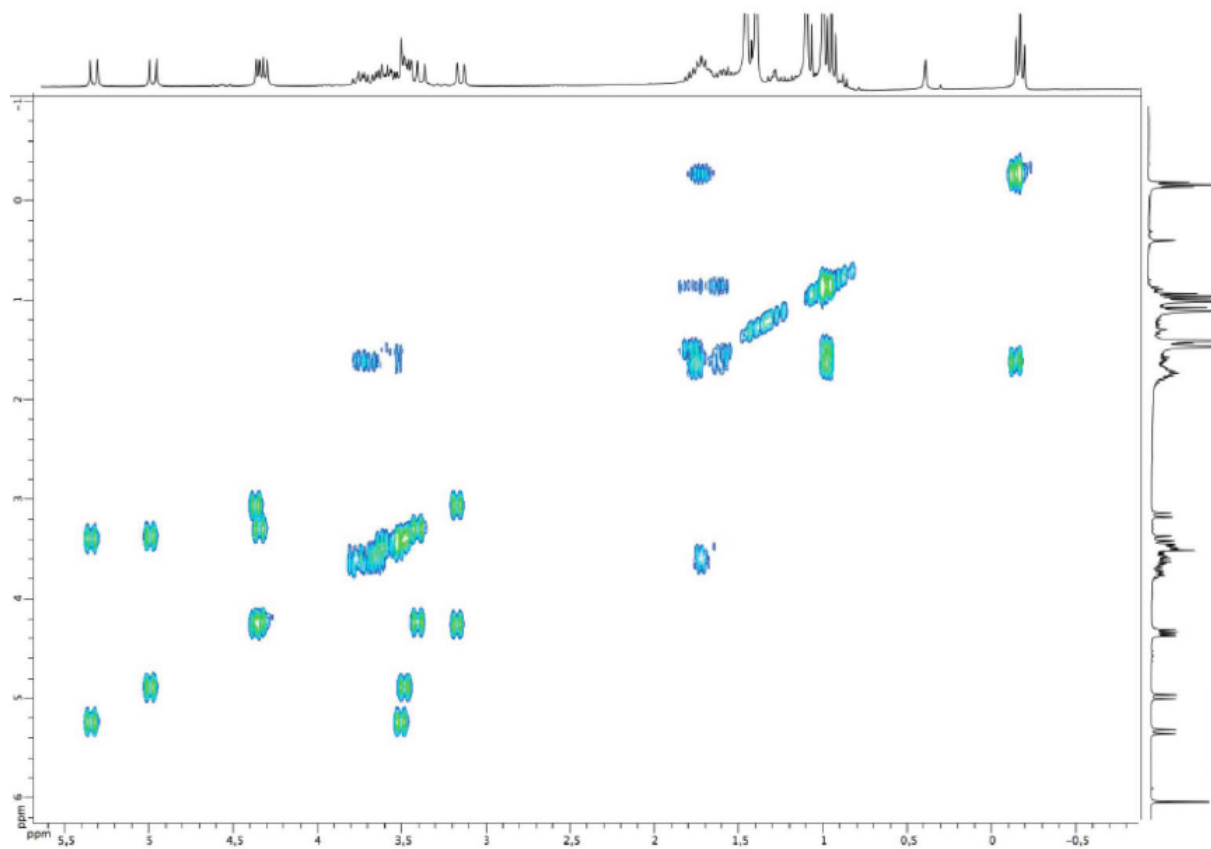
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**5,11,17,23-Tetra-*tert*-butyl-25,26-dipropoxy-27,28-dihydroxycalix[4]arene (4)**

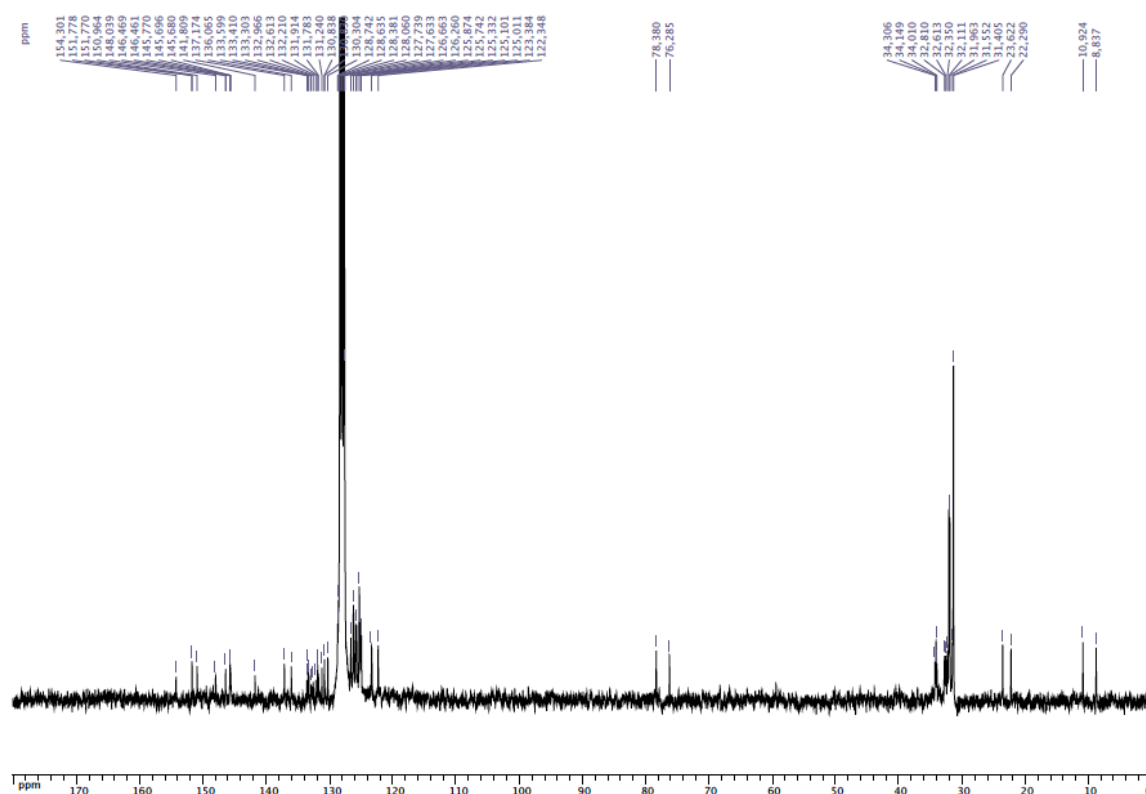


**(S,S)-5,11,17,23-Tetra-*tert*-butyl-25,26-dipropoxy-27,28-bis(1,1'-binaphthyl-2,2'-dioxyphosphanyloxy)calix[4]arene (3)**

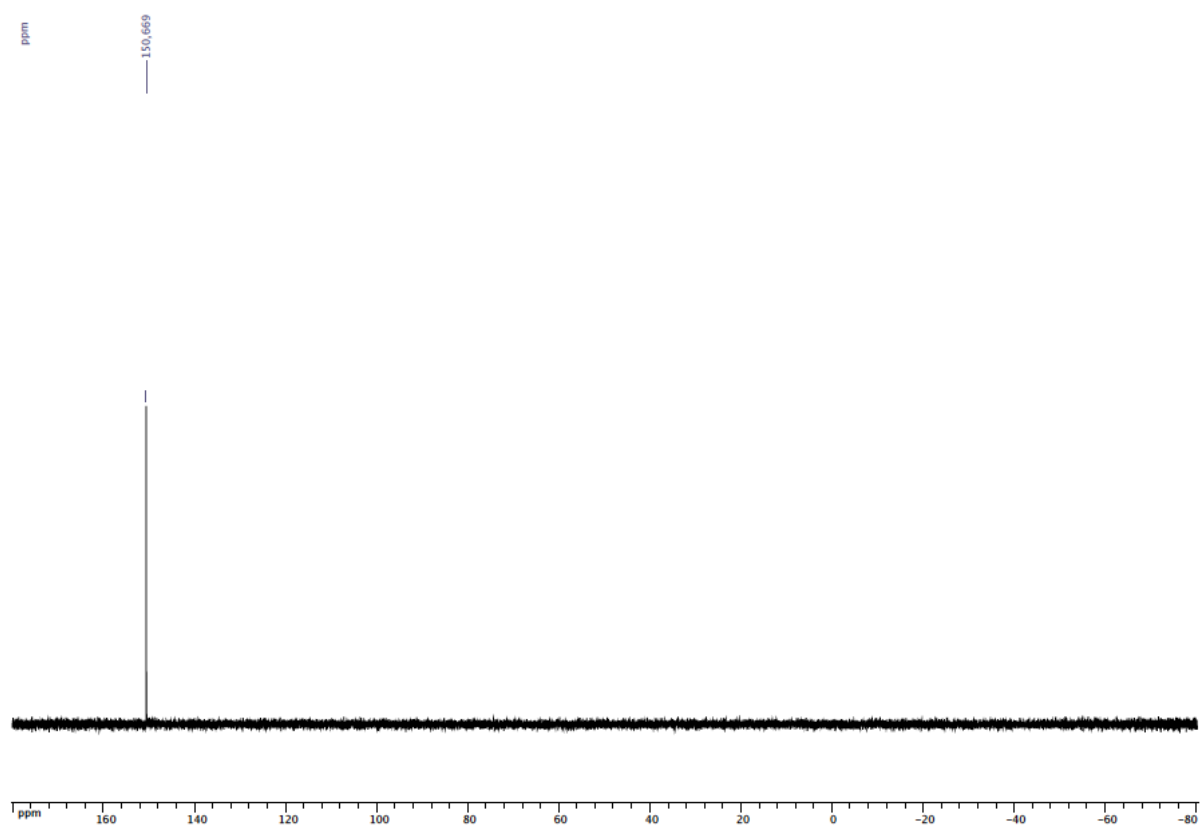
<sup>1</sup>H NMR spectrum (C<sub>6</sub>D<sub>6</sub>)



$^1\text{H}/^1\text{H}$  COSY spectrum ( $\text{C}_6\text{D}_6$ )

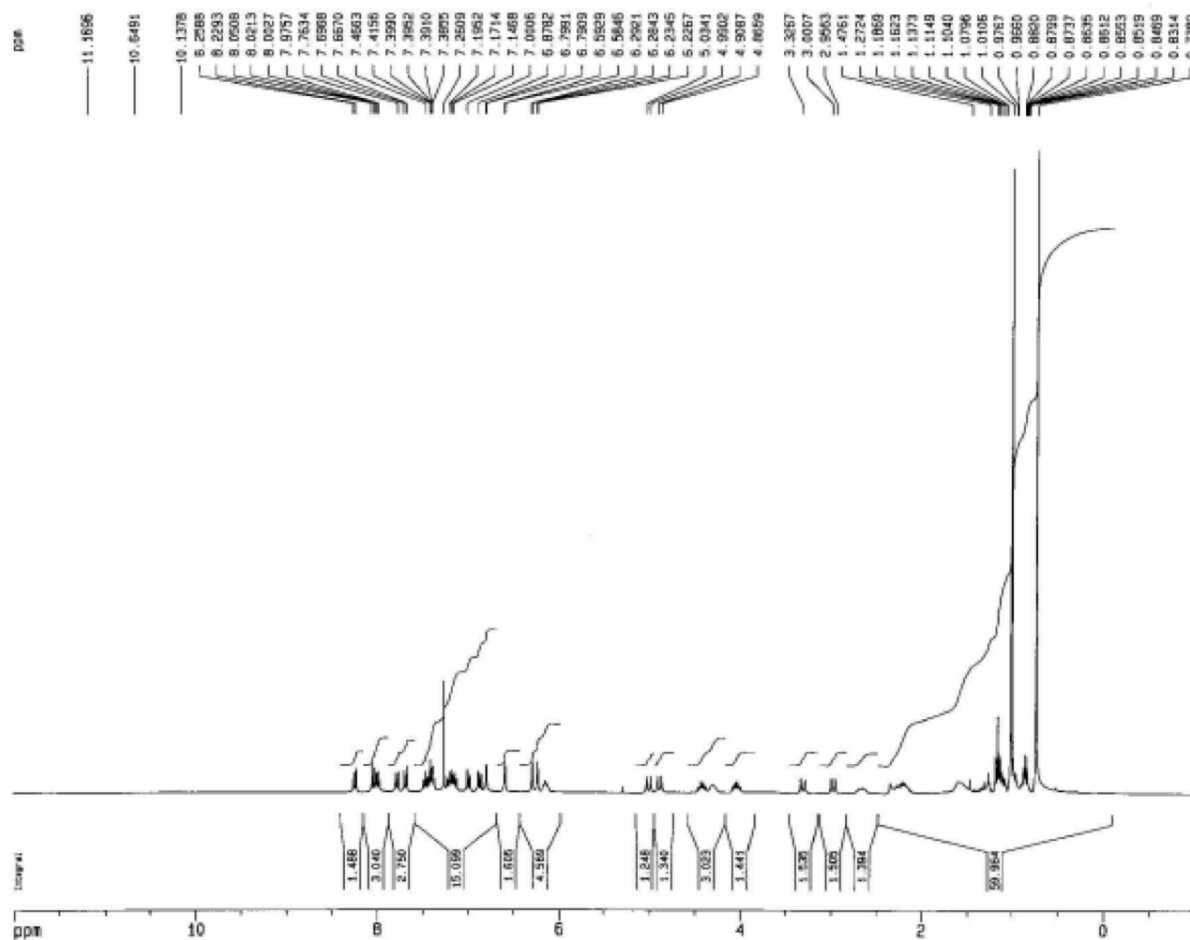
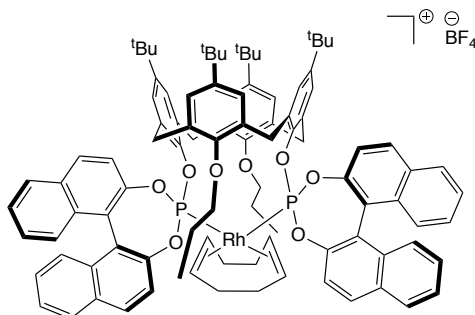


$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum ( $\text{C}_6\text{D}_6$ )

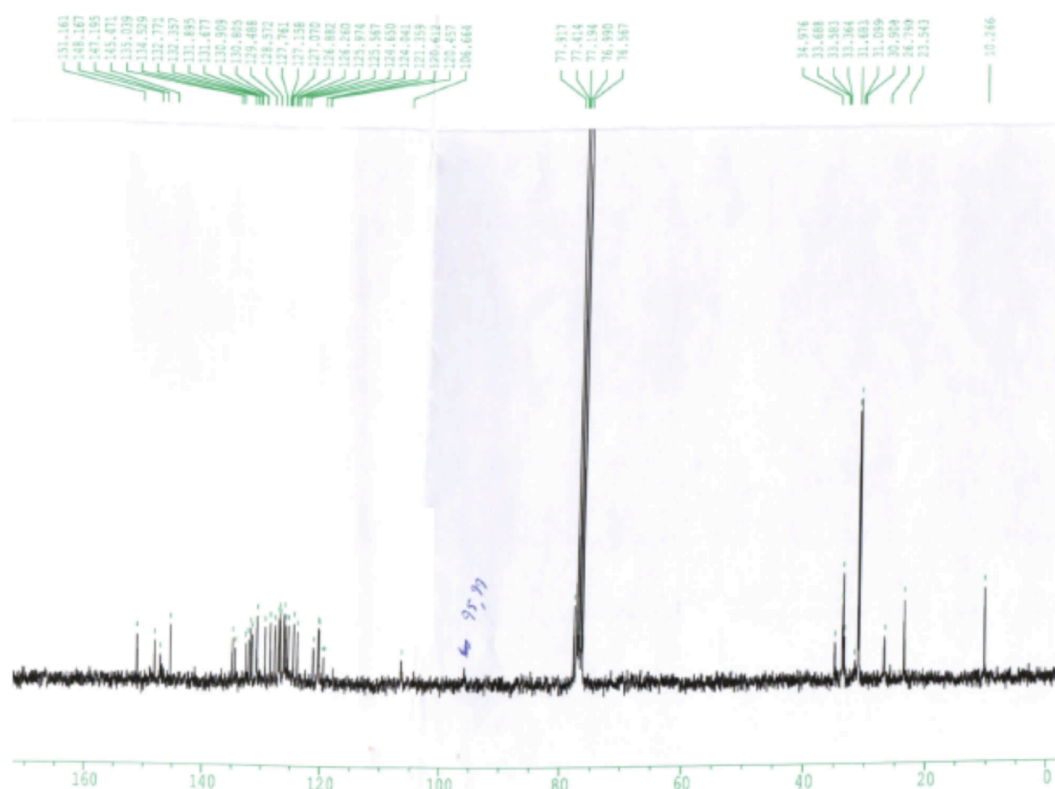


$^{31}\text{P}\{^1\text{H}\}$  NMR spectrum ( $\text{C}_6\text{D}_6$ )

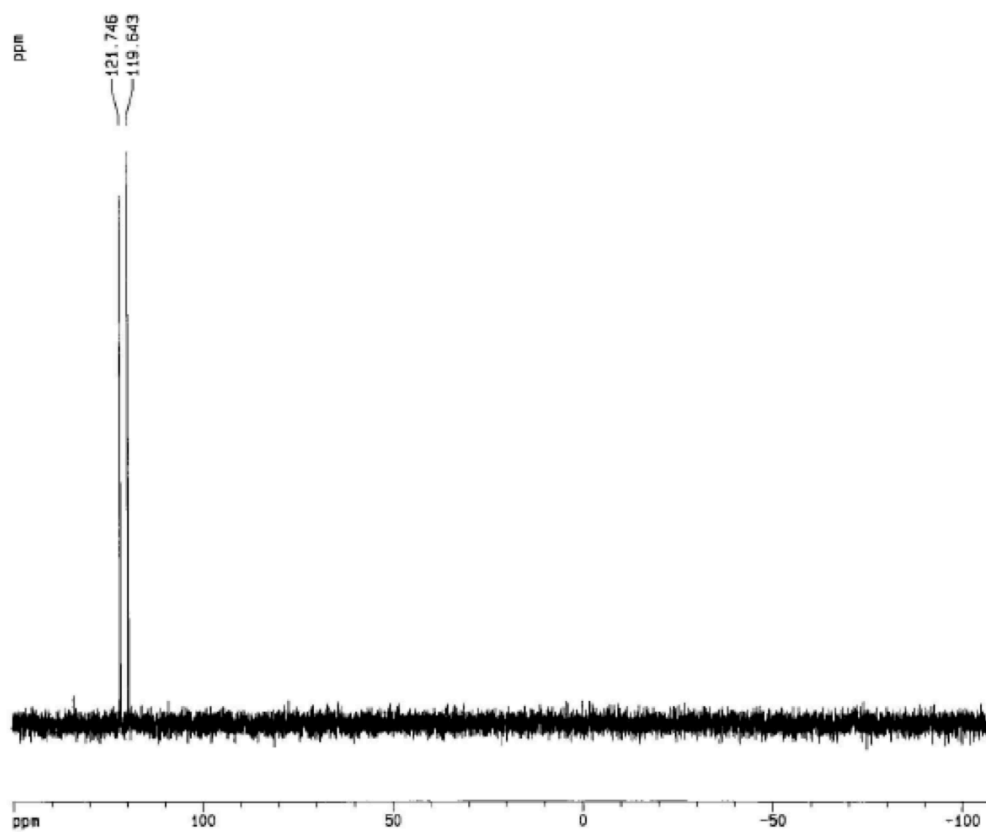
***cis-P,P'*-{[(*S,S*)-5,11,17,23-Tetra-*tert*-butyl-25,27-dipropoxy-26,28-bis(1,1'-binaphthyl-phosphite)calix[4]arene]-1,5-cyclooctadiene}rhodium(I) tetrafluoroborate (5)**



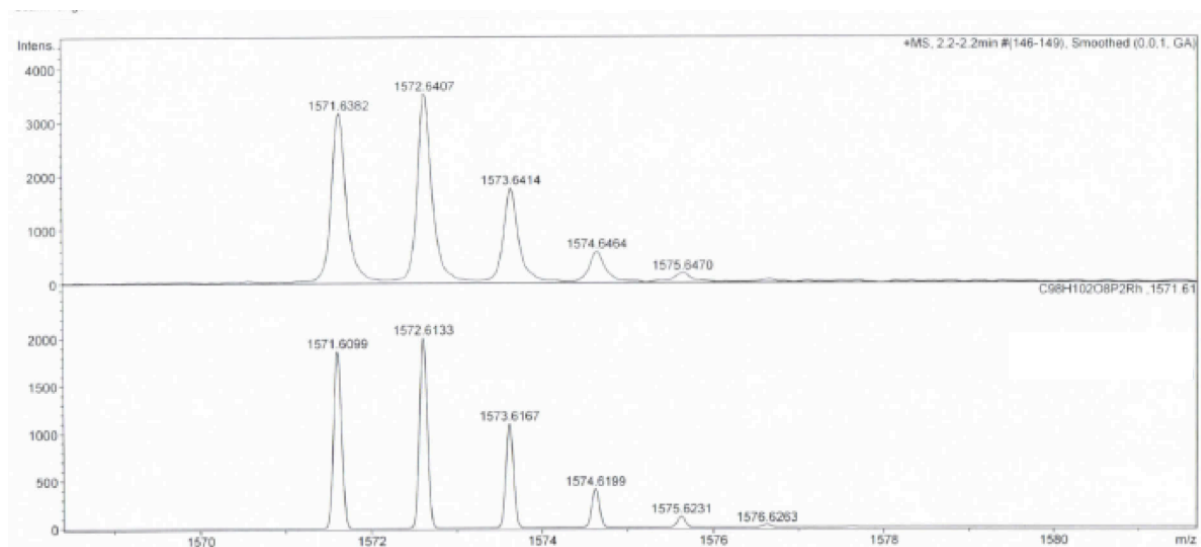
$^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ )



$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum ( $\text{CDCl}_3$ )



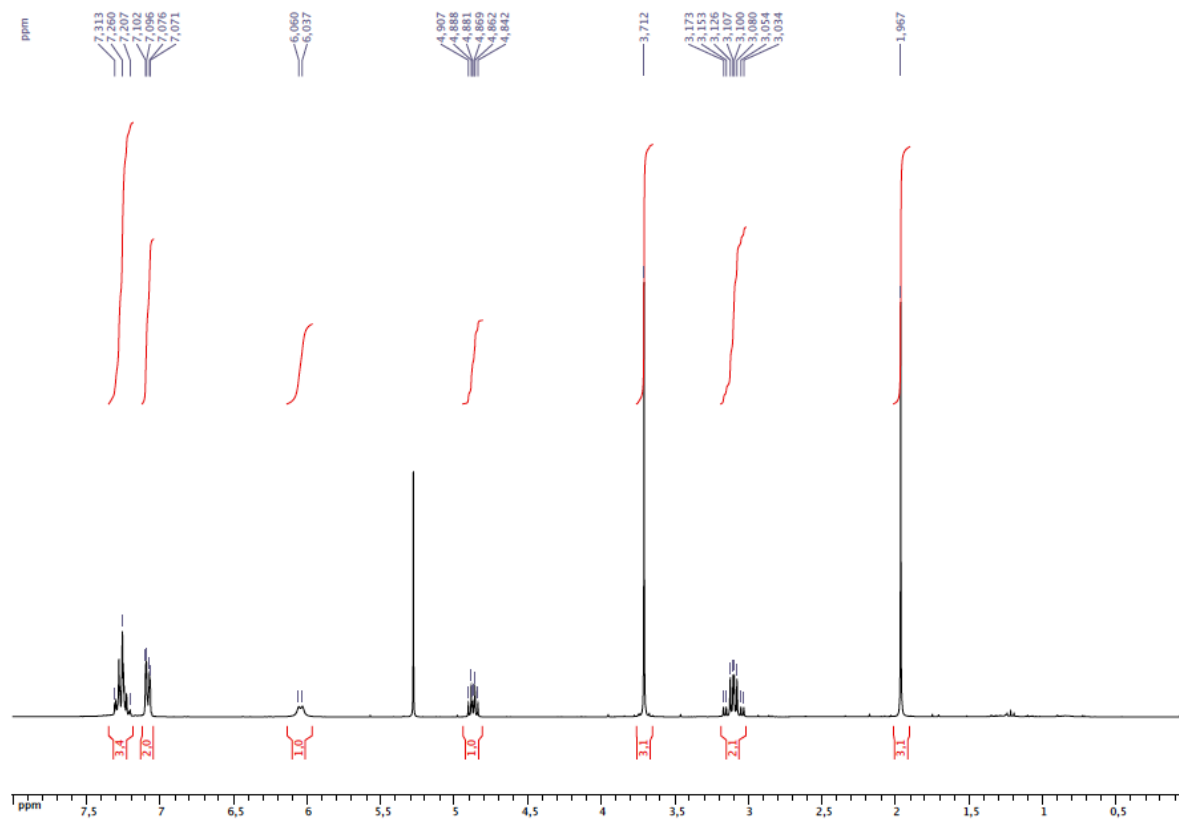
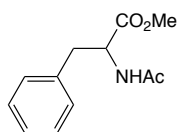
$^{31}\text{P}\{^1\text{H}\}$  NMR spectrum ( $\text{CDCl}_3$ )



Mass spectrum (ESI-TOF)  
exp. spectrum (top); calc. spectrum (bottom) for  $C_{98}H_{102}O_8P_2Rh$

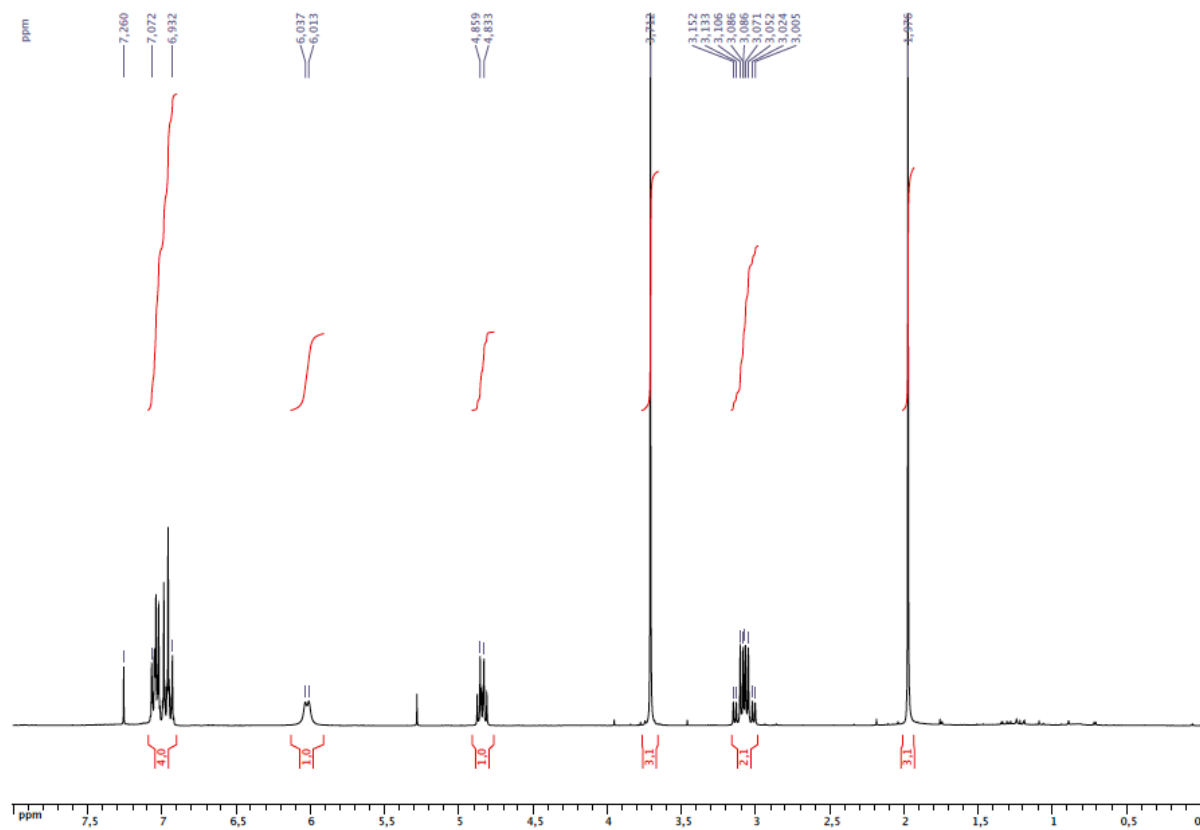
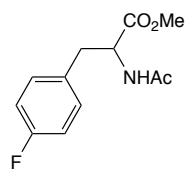


***N*-Acetyl-phenylalanine methyl ester (7a)**



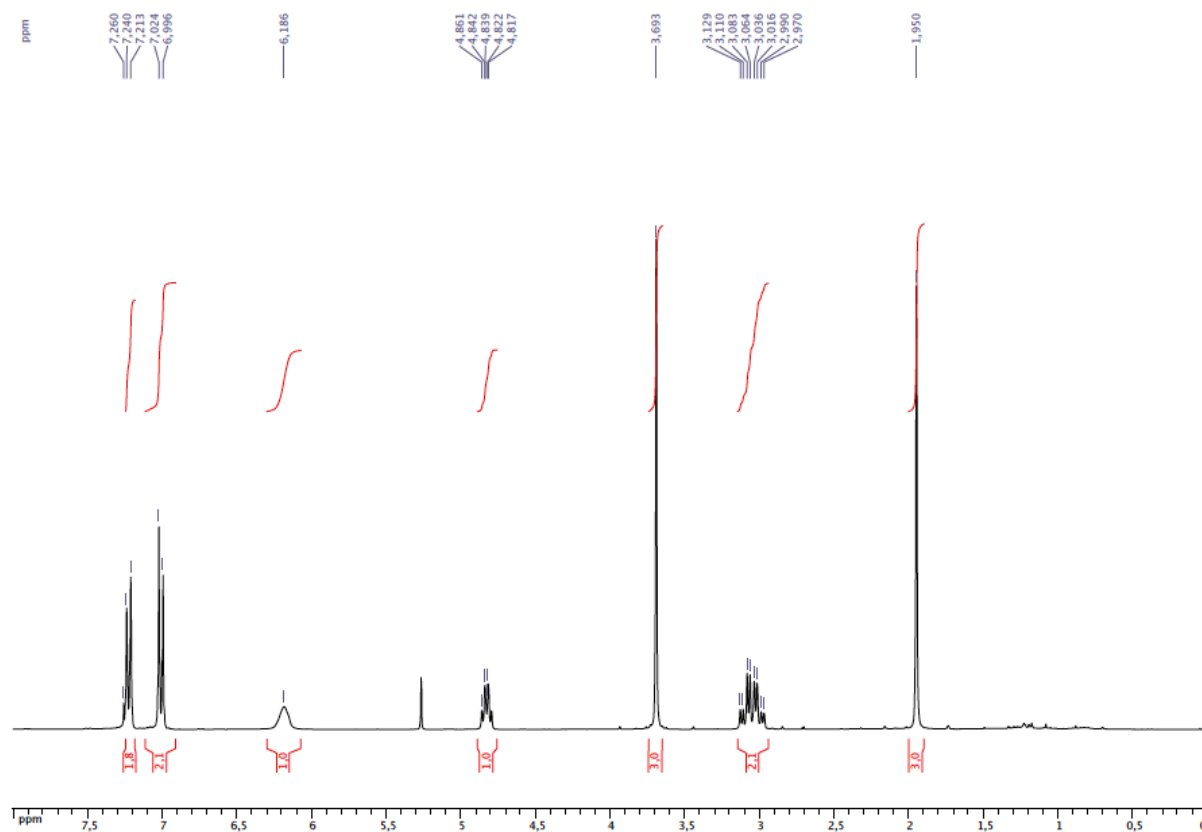
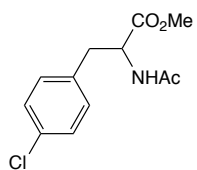
<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>)

***N*-acetyl-4-fluoro-phenylalanine methyl ester (7b)**

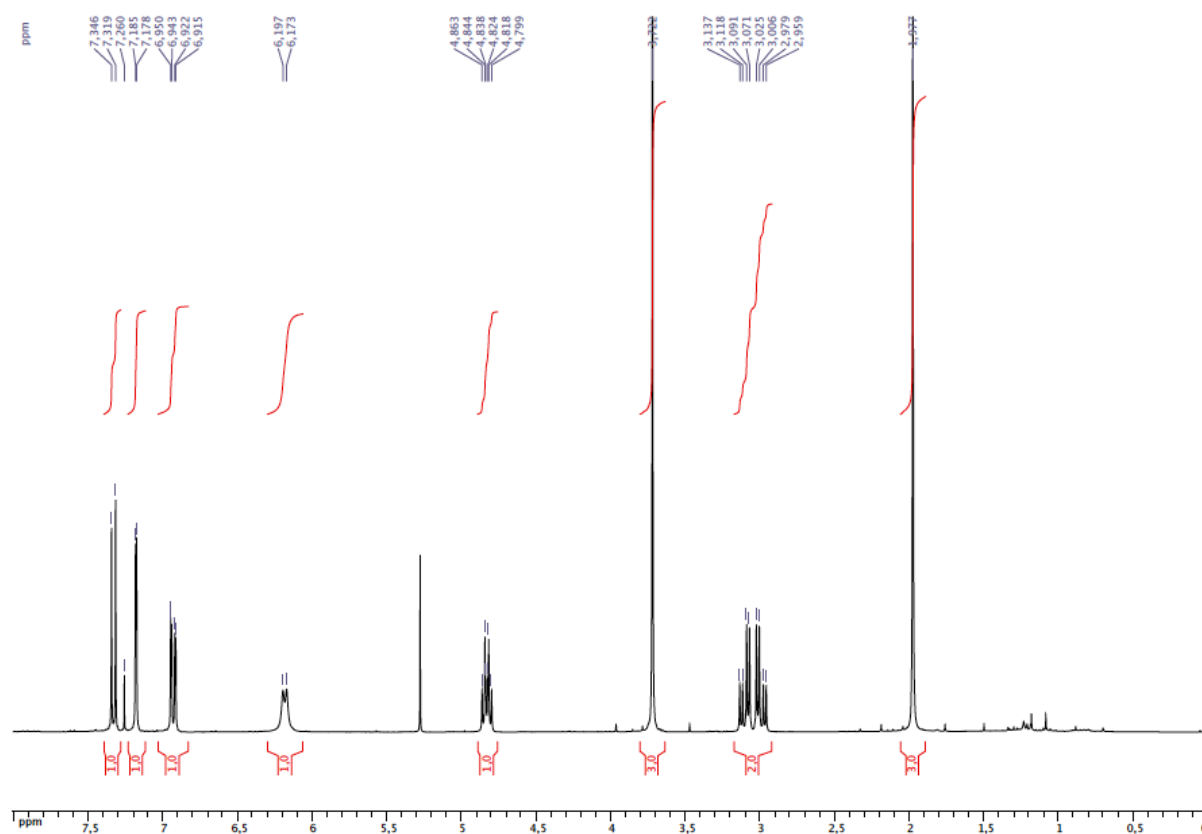
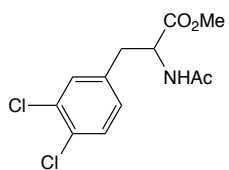


<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>)

***N*-Acetyl-4-chloro-phenylalanine methyl ester (7c)**



***N*-Acetyl-3,4-dichloro-phenylalanine methyl ester (7d)**



<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>)