New L-serine derivative ligands as co-catalysts for Diels-Alder reaction

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Supplementary data

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NMR spectra

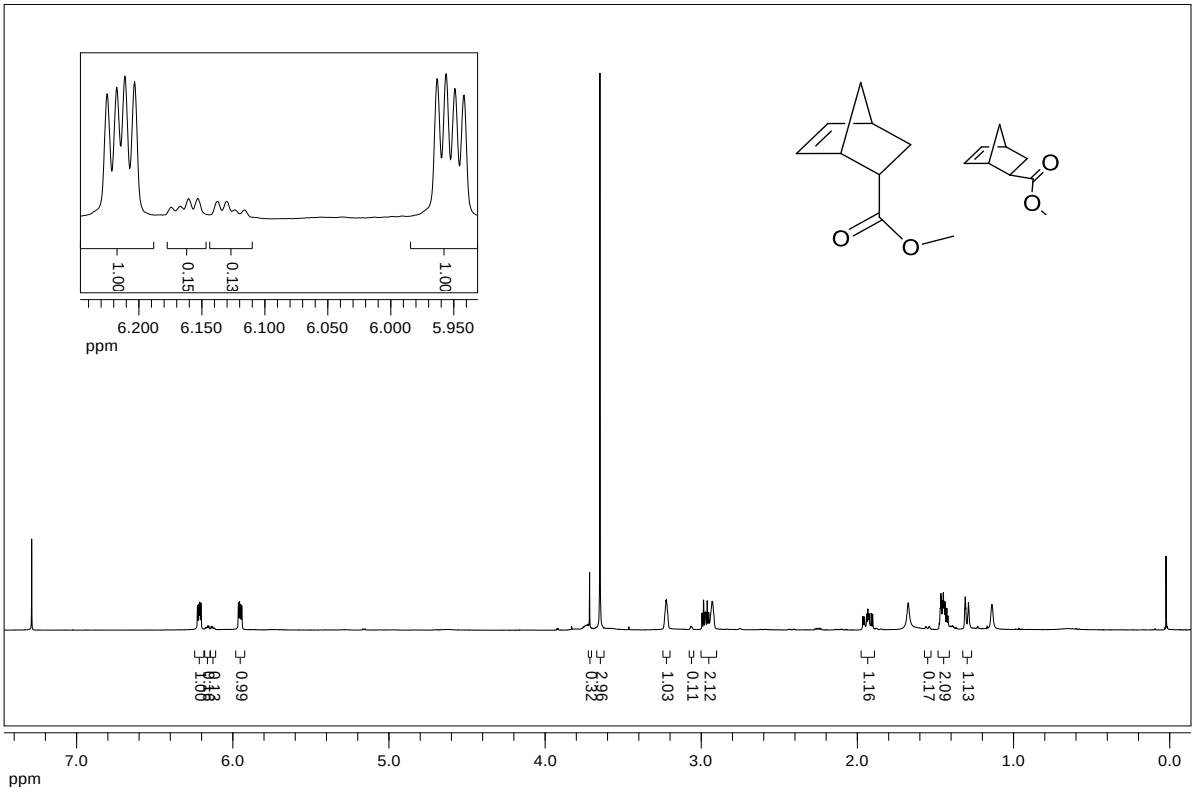


Fig. S1. ^{1}H-NMR spectra of a Diels-Alder reaction mixture catalyzed by ZnI_2, after extraction and evaporation of the volatiles, the **3-*endo*** adduct being majority over the **3-*exo***.

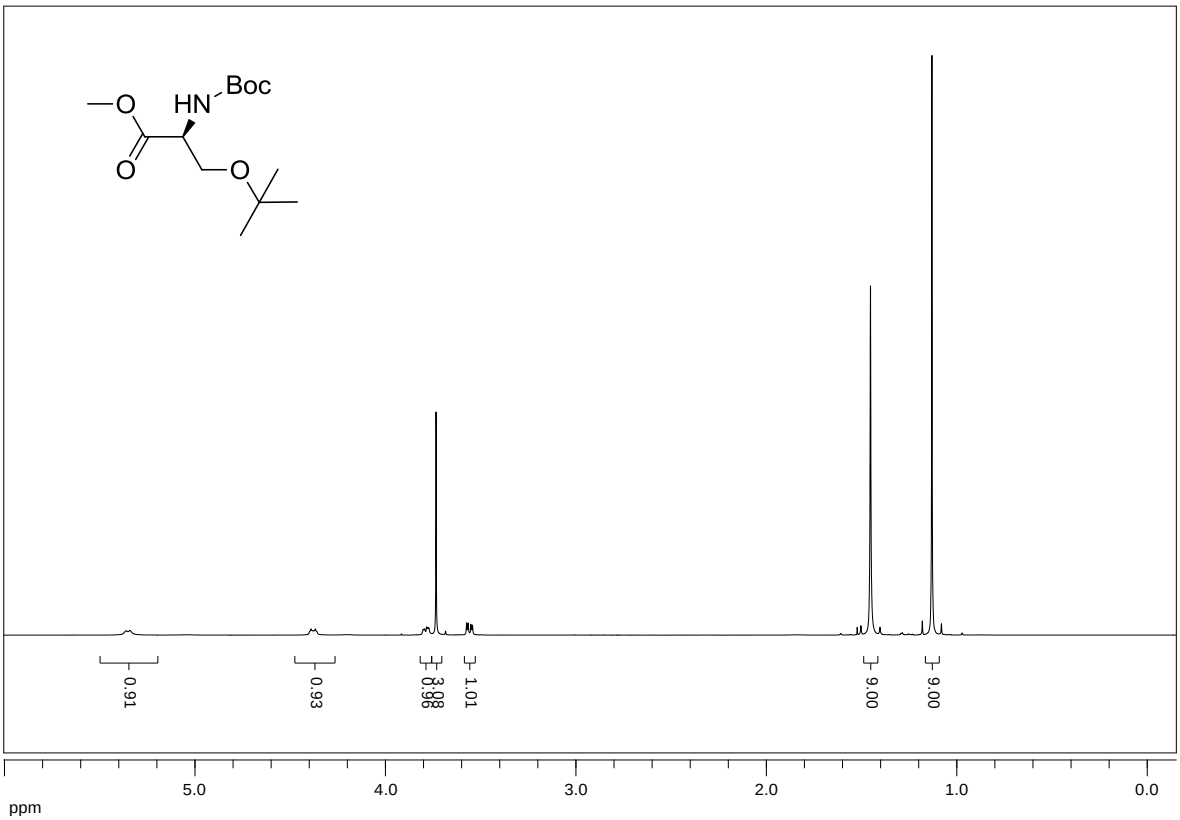


Fig. S2. ^{1}H-NMR spectra of ligand **4**.

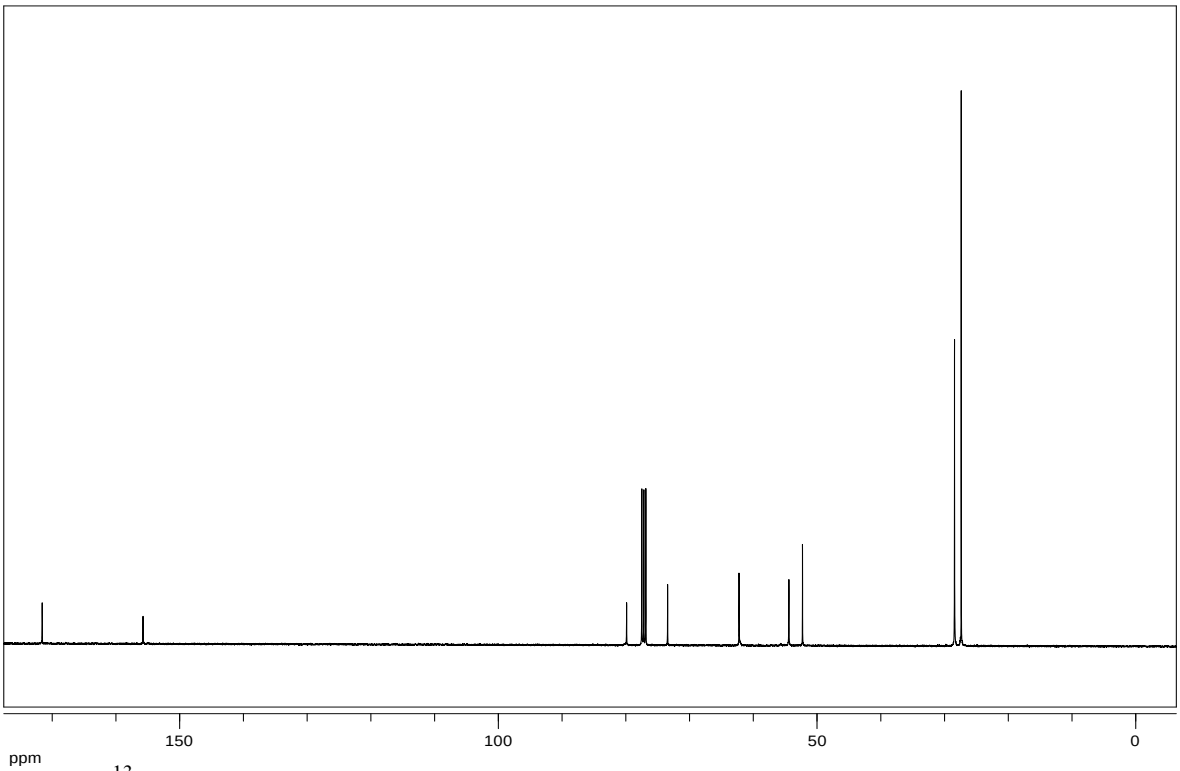


Fig. S3. ^{13}C-NMR spectra of ligand **4**.

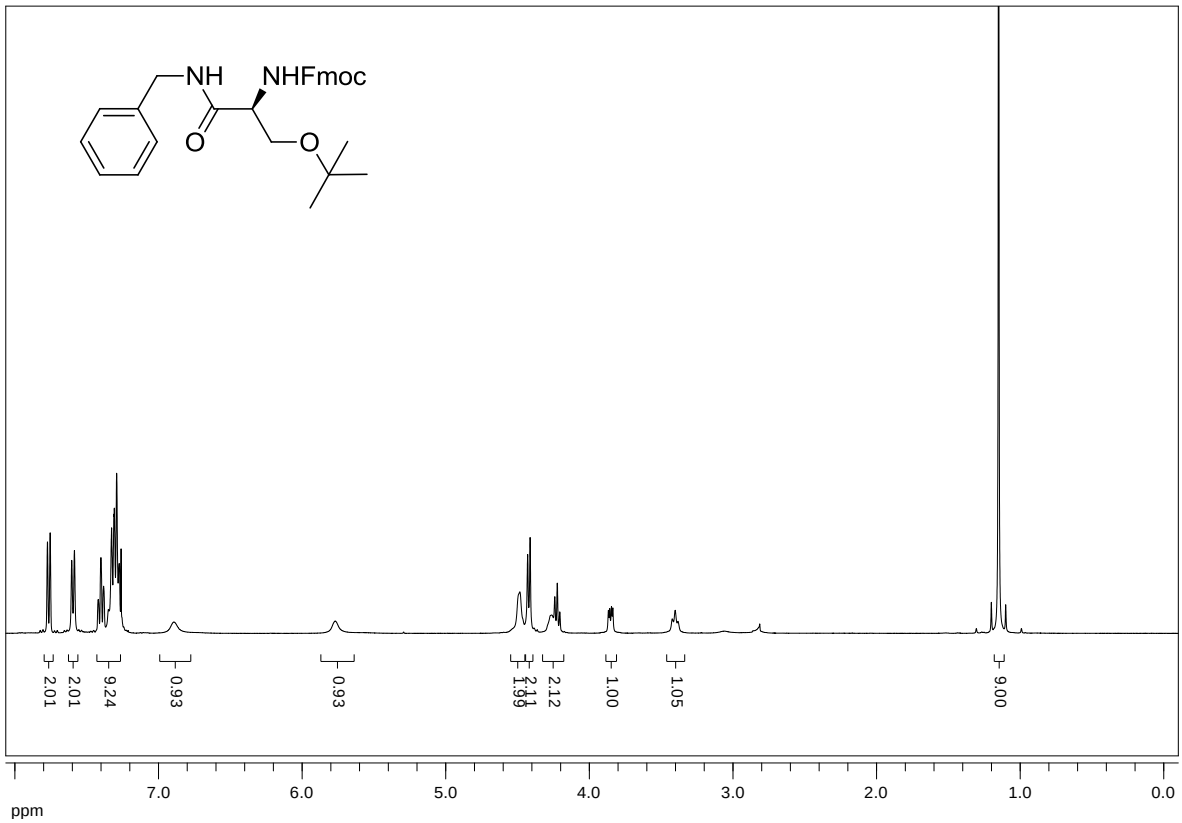


Fig. S4. ^{1}H-NMR spectra of serine derivative ligand **5**.

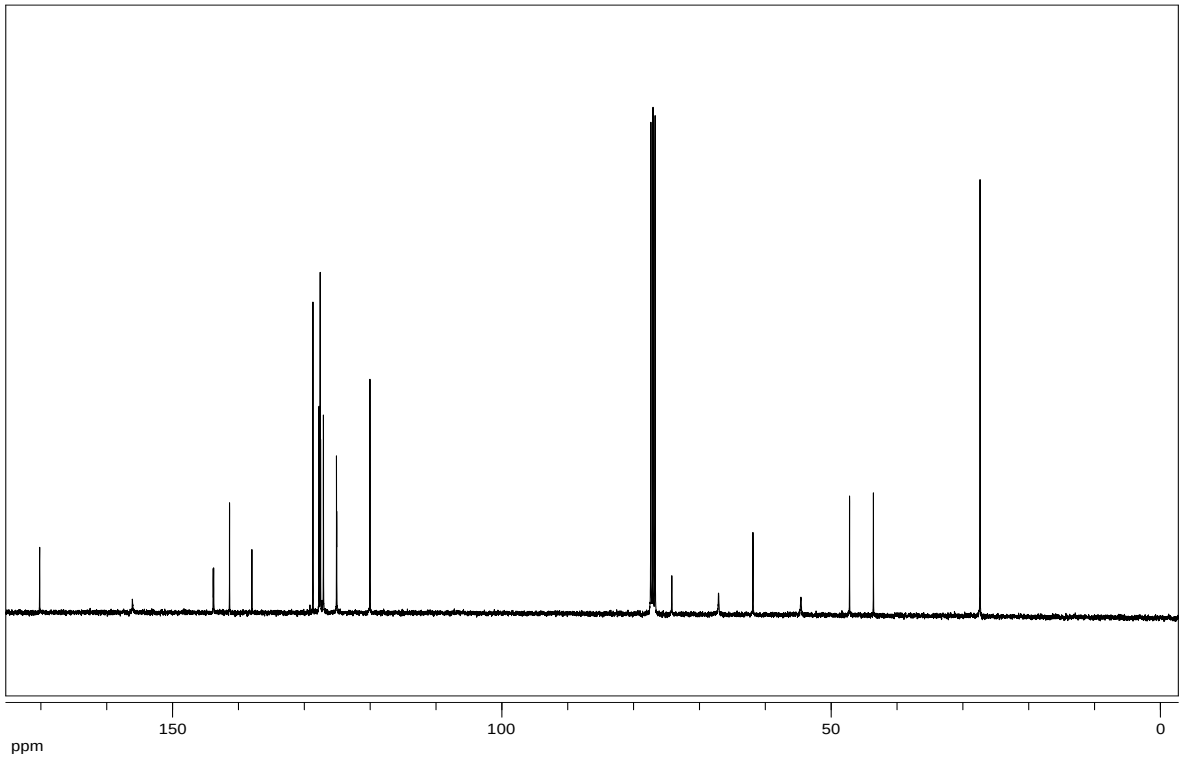


Fig. S5. ^{13}C-NMR spectra of serine derivative ligand **5**.

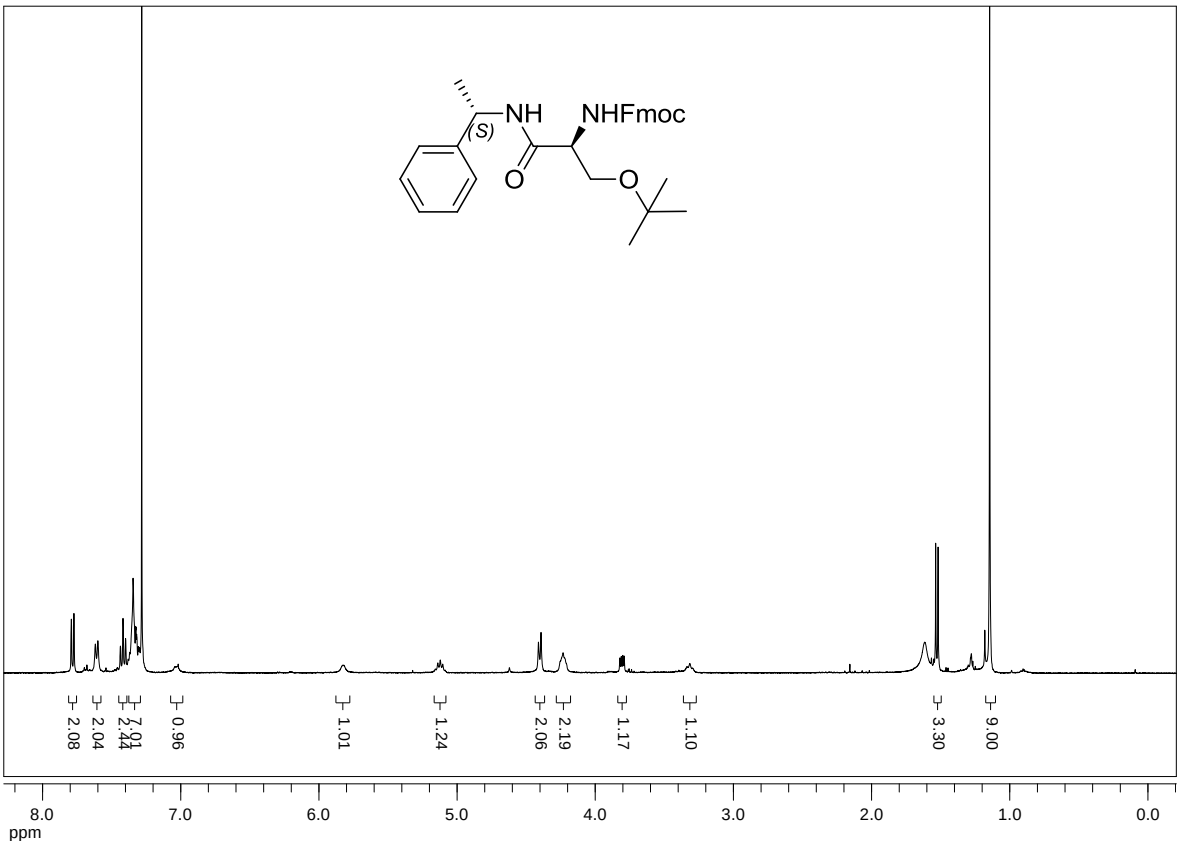


Fig. S6. ^{1}H-NMR spectra of serine derivative ligand **6**.

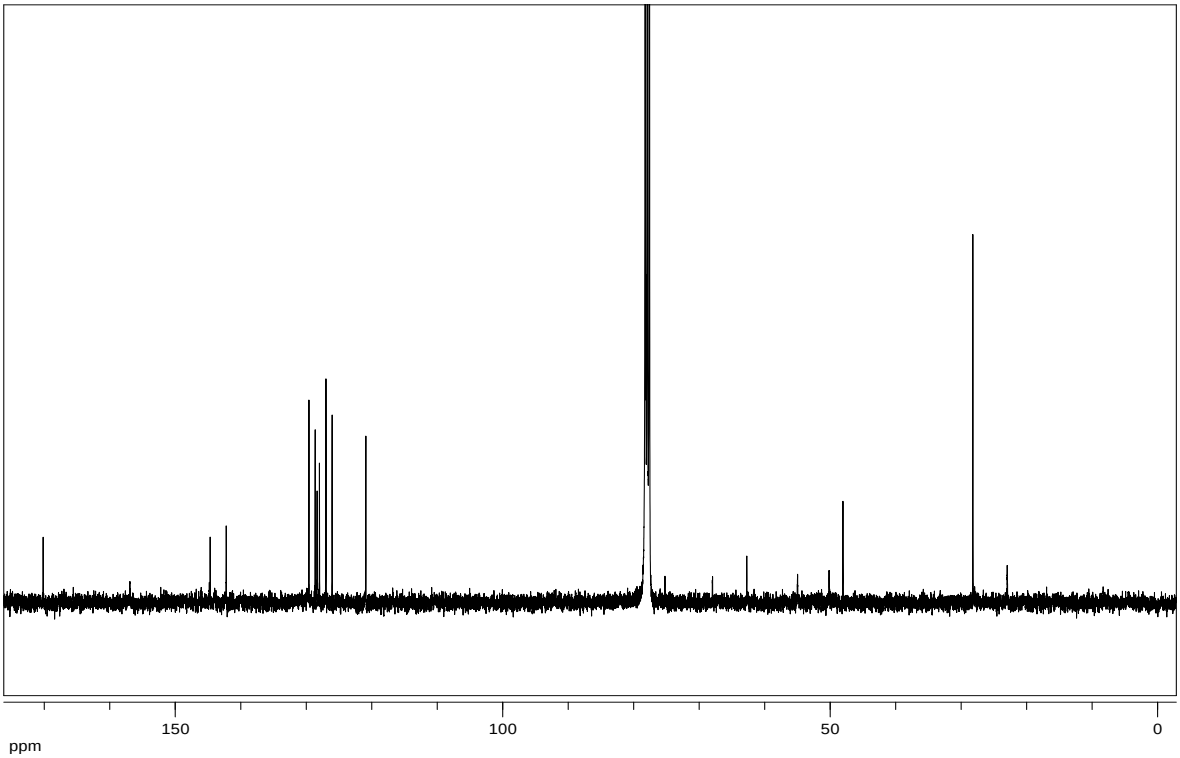


Fig. S7. ^{13}C-NMR spectra of serine derivative ligand **6**.

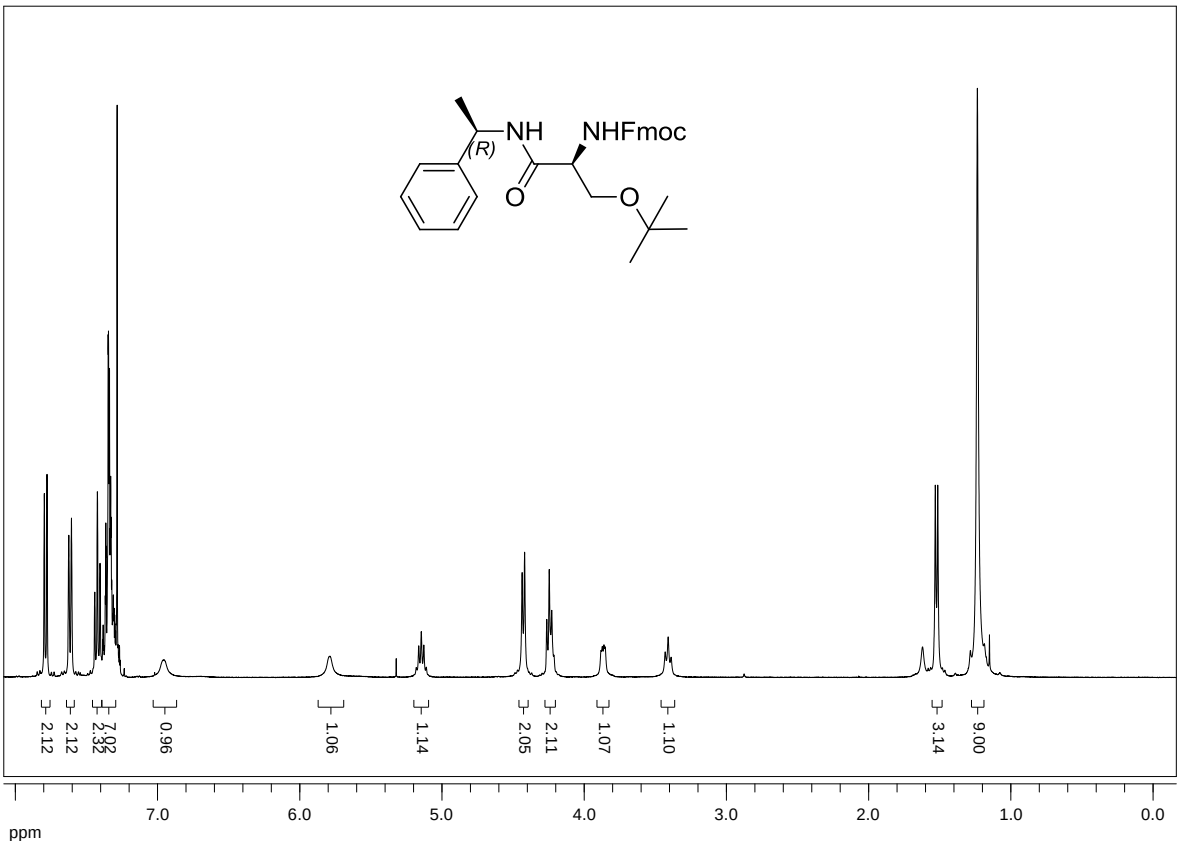


Fig. S8. ^{1}H-NMR spectra of serine derivative ligand **7**.

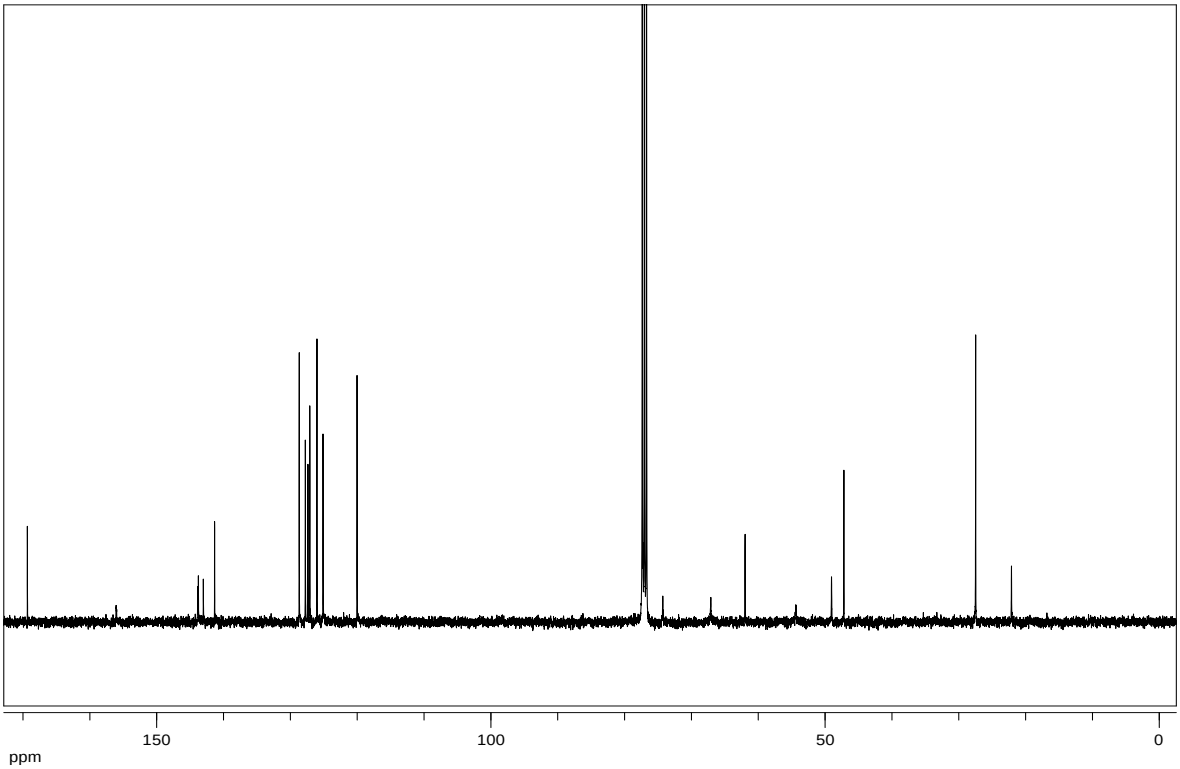
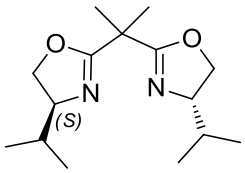


Fig. S9. ^{13}C-NMR spectra of serine derivative ligand **7**.

Diels-Alder reactions using BOX ligands as co-catalysts



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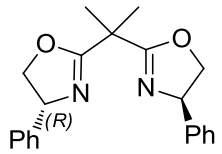

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Fig. S10. Structure of BOX ligand **4**, 2,2-bis((4*S*)-4-isopropyloxazoline)propane and **5**, 2,2-bis((4*R*)-4-phenyloxazoline)propane, tested as co-catalysts in Diels-Alder reaction between CPD and methyl acrylate.

Table 2. Results of the the Diels-alder reaction between CPD and methyl acrylate, yield, *endo*/*exo* ratio of adduct **3** and enantiomeric excess (e.e.) using BOX ligands **11** and **12**.

entry	**catalyst**	**ligand**	**η / %**	***endo*/*exo* ratio** [a]	**e.e. / %** [b] (configuration)
1	$Cu(OTf)_2$	**11**	16	83/17	87 (*R*)
2	ZnI_2	**11**	10	86/14	34 (*R*)
3	$Cu(OTf)_2$	**12**	58	83/17	18 (*R*)
4	ZnI_2	**12**	13	83/17	28 (*R*)
5	$Cu(OTf)_2$[c]	**12**	23	84/16	12 (*R*)

The reactions were performed with 10 % of both catalyst and ligand during 20 h, the temperature allowed to rise from 0 ºC to room temperature, following the procedure described before. *a*- measured by ^{1}H-NMR; *b*- measured by chiral GC; *c*- 15% of ligand and 10% of catalyst, during 20 h, were used.