Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Regioselective Monochloro-substitution in Carbohydrates and Non-sugar Alcohols *via* Mitsunobu Reaction: Applications in the Synthesis of Reboxetine

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SUPPORTING INFORMATION

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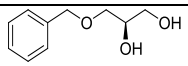
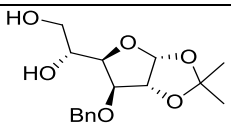
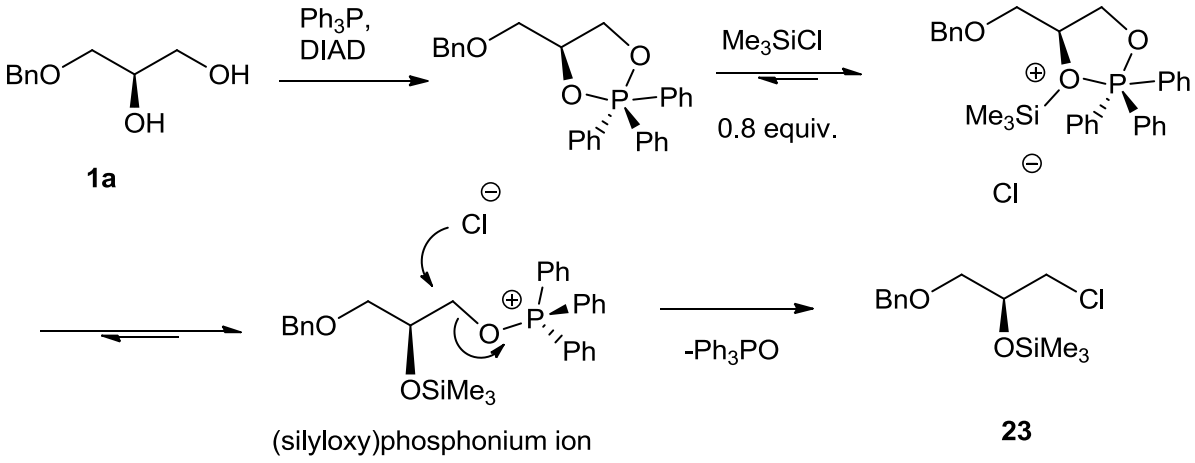
Section A: List of known compounds and their references

Entry	Compound No. in Manuscript	References
1.	**1a**	*Tetrahedron: Asymmetry* **2011**, *22*, 658–661.
2.	**2a,3a**	*Heterocycles* **1991**, *32*, 1587.
3.	**4a**	*Tetrahedron: Asymmetry* **2009,** *20*, 2287–2292.
4.	**1b**	*Bioorganic & Medicinal Chemistry letters*, **1997**, *7*, 225-228.
5.	**4b**	Patent-WO 02/092602 A2
6.	**1c**	*Tetrahedron: Asymmetry* **2008,** *19*, 1455-1460.
7.	**1d**	*Organic Letters* **2012**, *14*, 2626
8.	**2d**	*Synthesis* **2006**, 1427. *Tetrahedron: Asymmetry* **2006**, *17*, 1561-1567.
9.	**3d**	*J. Org. Chem*. **2012**, *77*, 1722-1737.
10.	**1e**	*Tetrahedron* **2009**, *65*, 2966-2974.
11.	**3e**	*Journal of Chemical Research, Synopses* **1987**, *12*, 400-401.
12.	**1g**	*Tetrahedran* **1985**, *41*, 1393-1399.
13.	**1h**	Patent-JP 1992-315212, 19921125. PCT WO93/05763
14.	**3h**	*Eur. J. Org. Chem.* **2007,** 2100-2106.
15.	**1i**	*Tetrahedron letters* ***2006***, *47*, *5285* *Journal of Molecular Catalysis A: Chemical* **2005,** *238*, 229–232.
16.	**1j**	*Helvetica Chimica Acta* **1964**, *47*, 398-407. *Organic Letters* **2012,** *14*, 2142–2145.
17.	**3j**	*Carbohydrate Research* **1988,** *177*, 247-252.
18.	**1k**	*Journal of Molecular Catalysis A: Chemical* **2005,** *238*, 229–232. *Synlett* **2000**, 110-112. *Tetrahedron Letters* **2005,** *46*, 7439-7441.
19.	**1l**	*Carbohydrate Research* **2004**, 339, 385–392. *J. Chem. Soc., Perkin Trans*. 1 **1998**, 1069–1080.
20.	**1m**	*J. carbohydrate chemistry*, **1998,** *17*, 439-452.
21.	**1n**	*Carbohydrate Research* **2004**, *339*, 385–392. *J. Chem. Soc., Perkin Trans. 1* **1998**, 1069–1080.
22.	**3n**	*Journal of Organic Chemistry* **2002**, *67*, 3733-3741.
23.	**14**	*Agric. Biol. Chem*. **1984**, *48*, 1841-1844.
24.	**15**	*Chem. Eur. J.* **2009**, *15*, 1713 –1722.
25.	**1g**	*Tetrahedran* **1985**, *41*, 1393-1399.
26.	**18**	*Green Chem. 2012,14, 123-129*
27.	**19**	*Tetrahedron: Asymmetry* **2012,** *23*, 650–654.
28.	**20**	Patent- *Offenlegungsschrift* 2921973, **1980**.

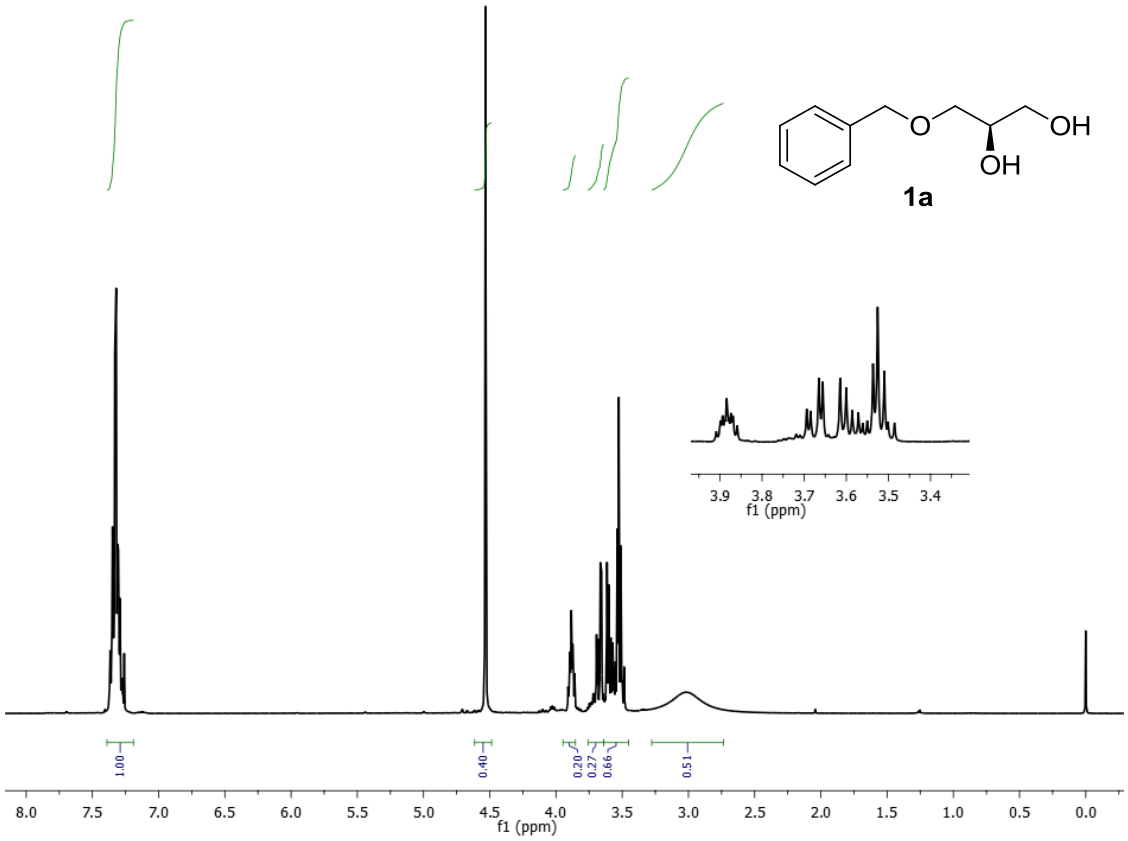
Table 1. Optimization of solvents for Mitsunobu reaction

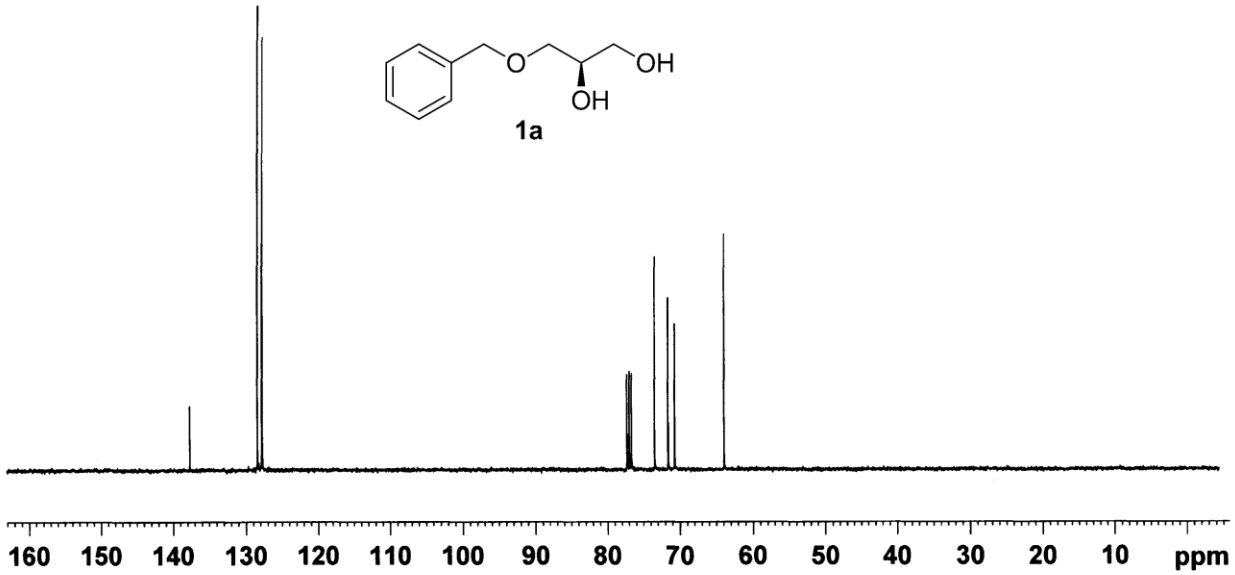
Entry	Substrate	Solvent	Time (h)	Product (%)
1		DCM	3	88
2		THF	2.5	85
3		Toluene	2	92
4		DCM	3	92
5		THF	3	92
6		Toluene	2	95

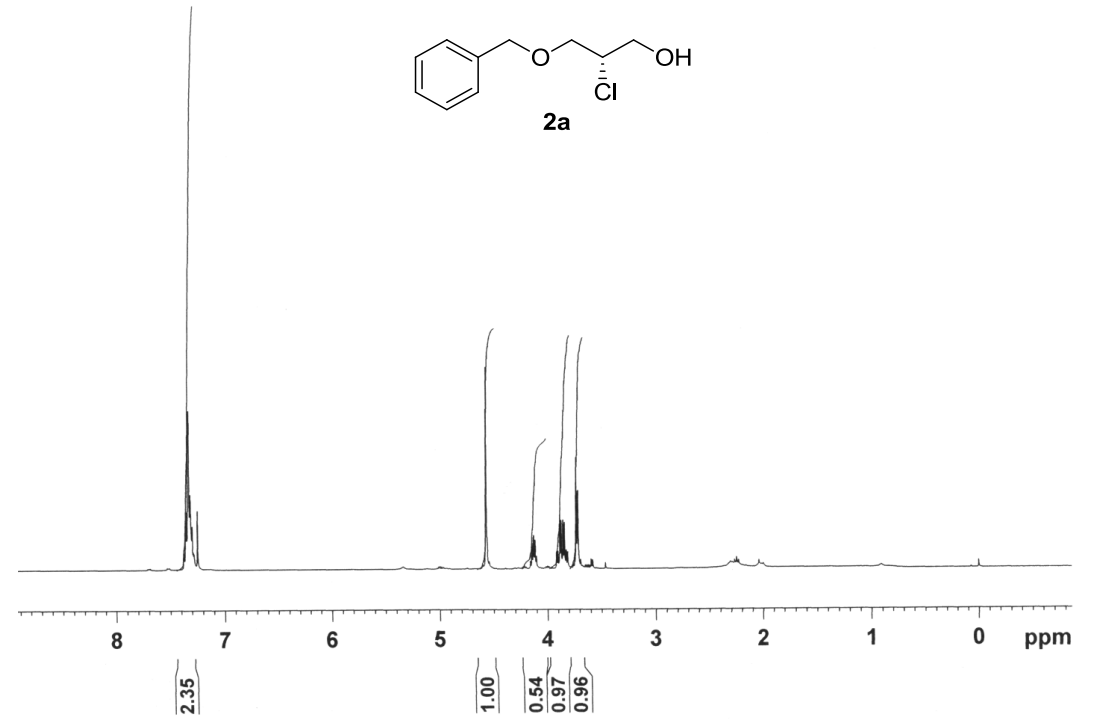


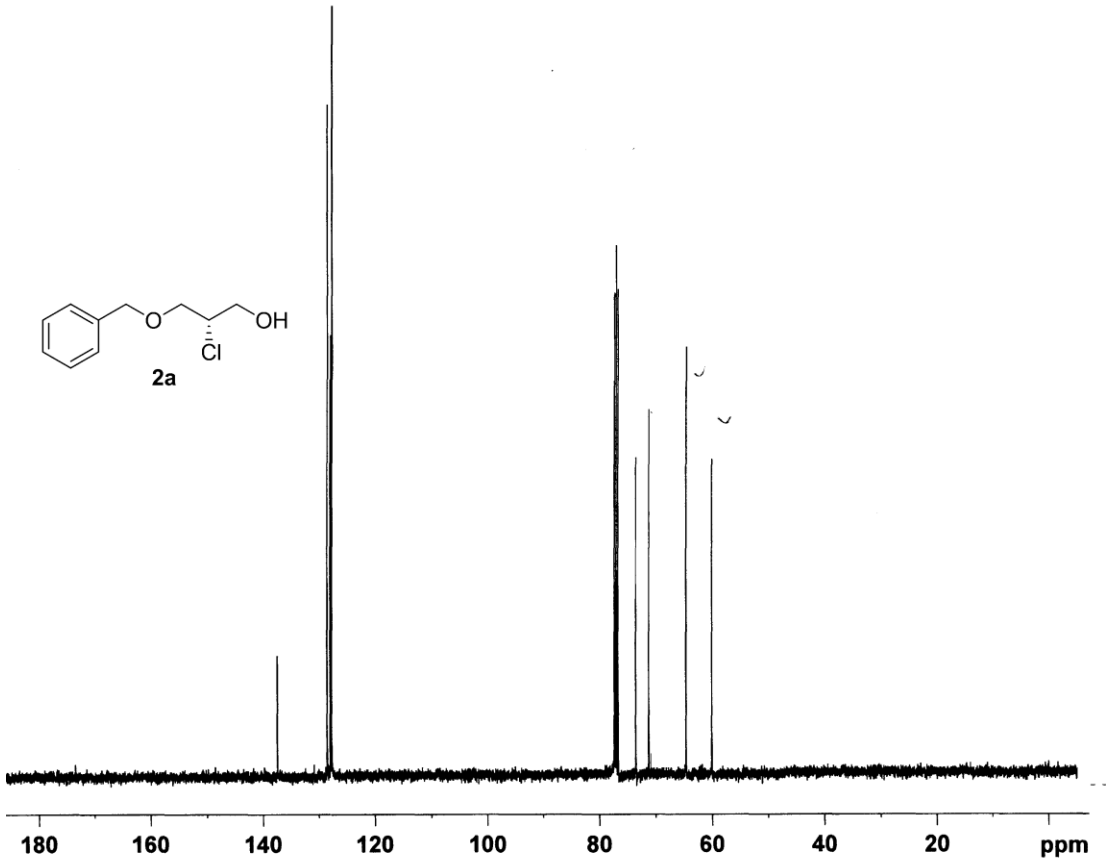
Scheme 1. Mitsunobu reaction in (*R*)-3-(benzyloxy)propanediol

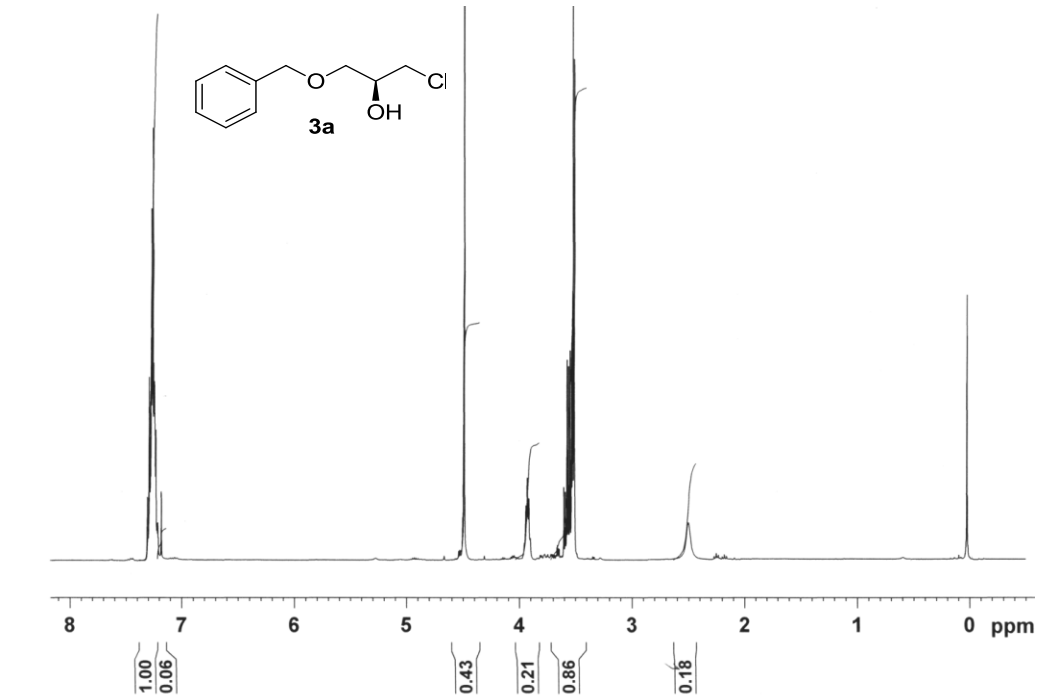
Section B: Copies of ^{1}H NMR, ^{13}C NMR Spectra

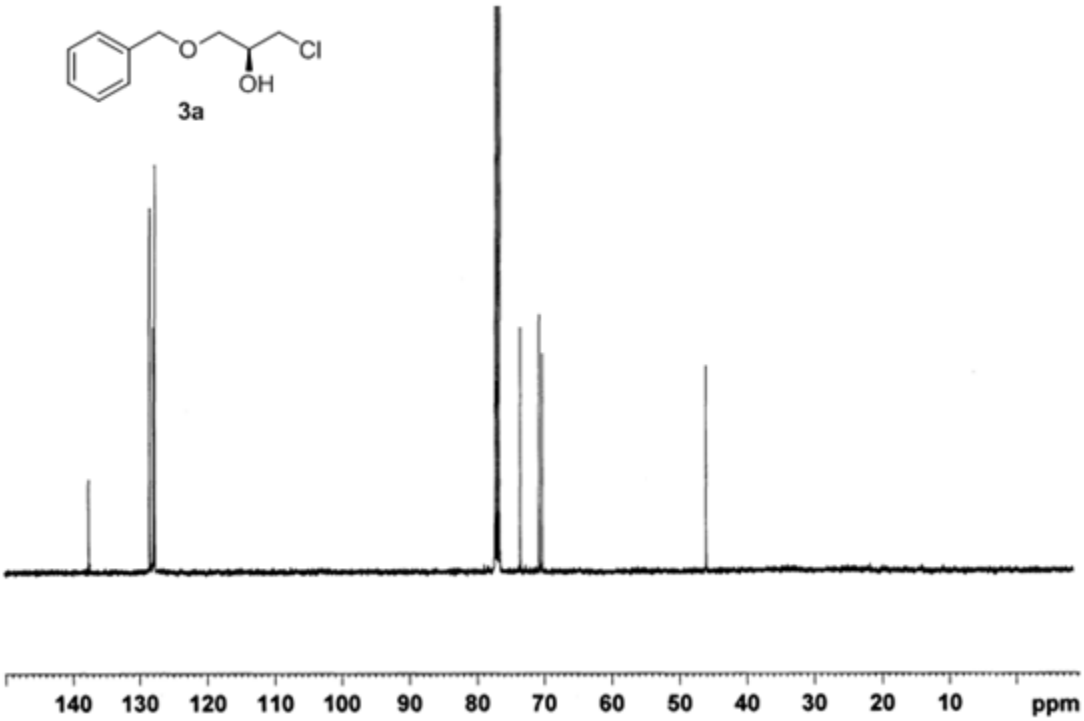


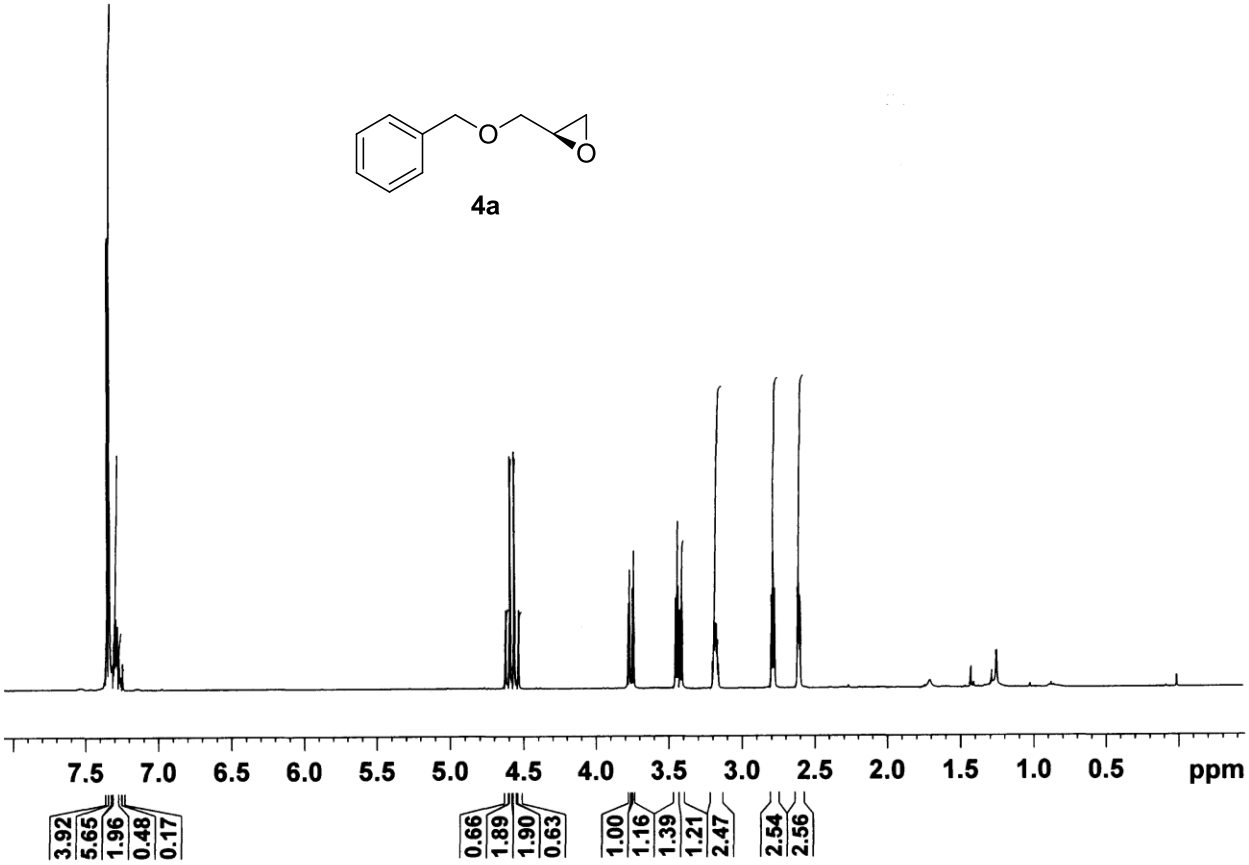


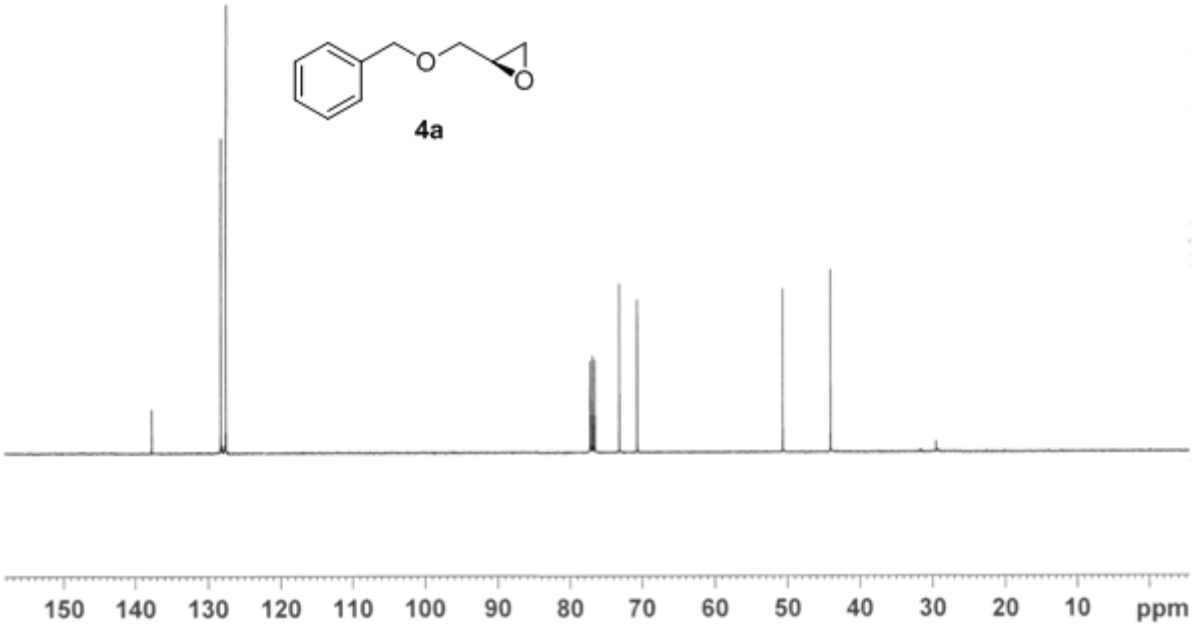


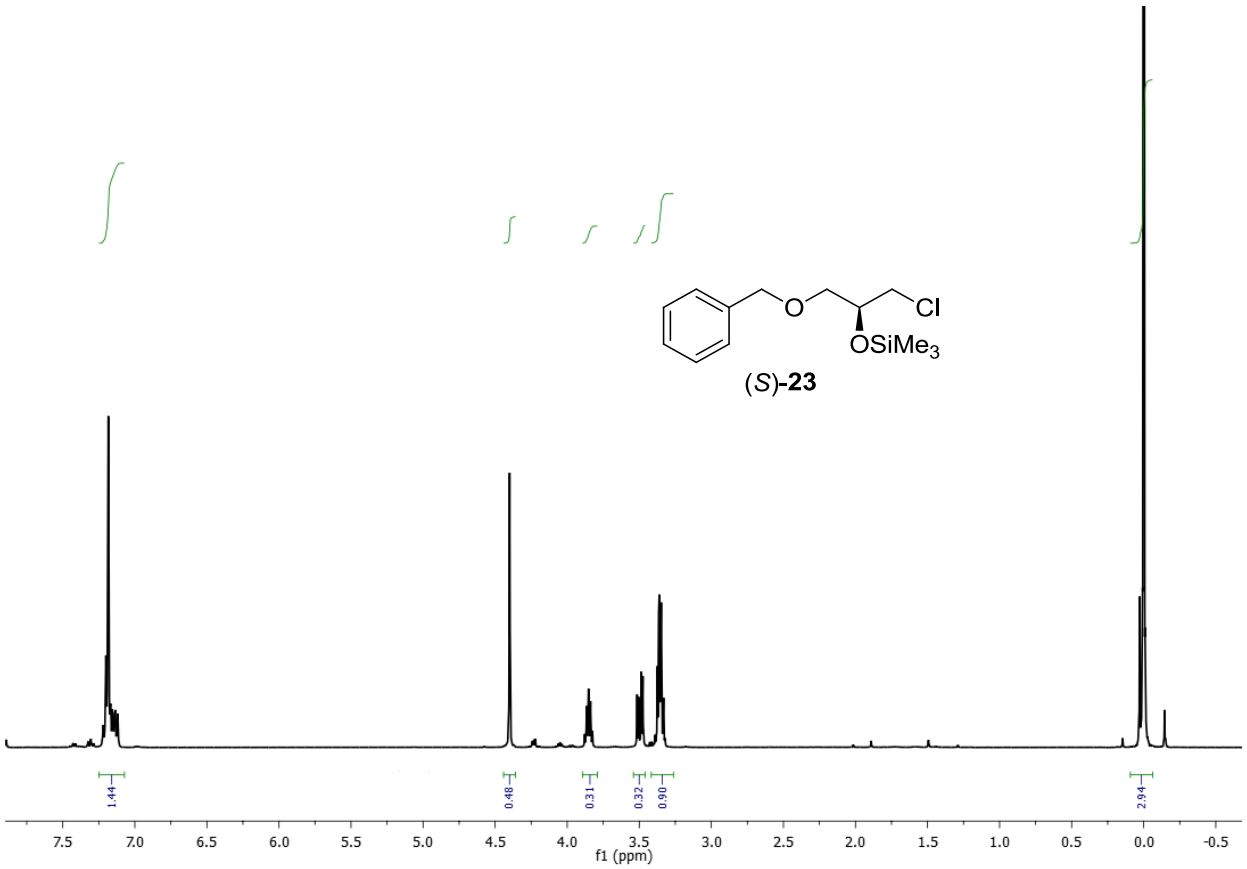




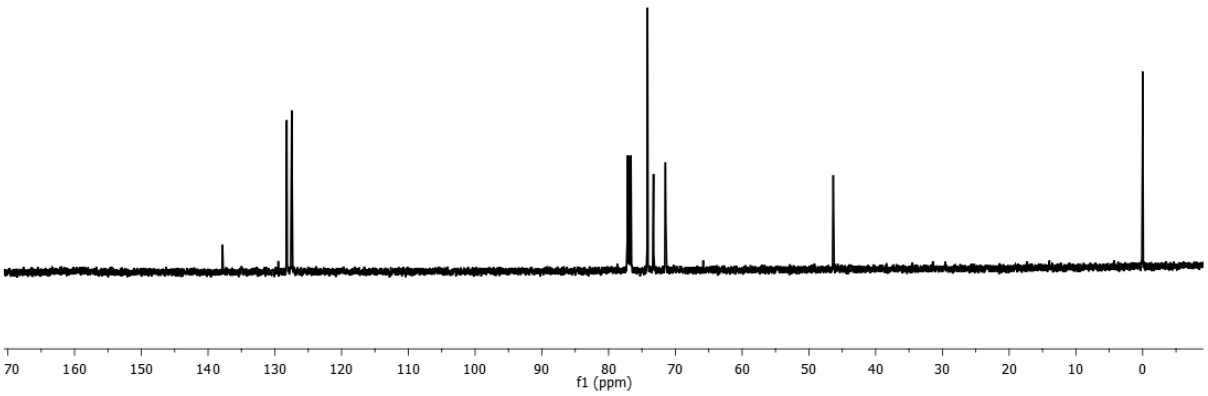


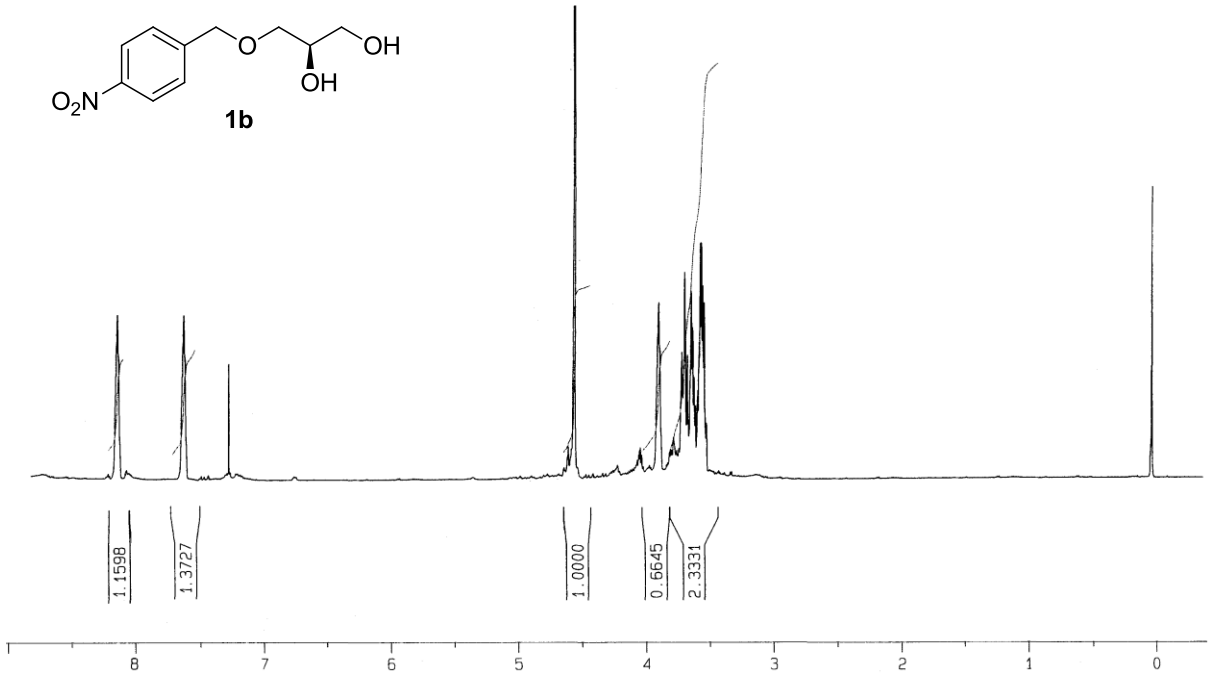


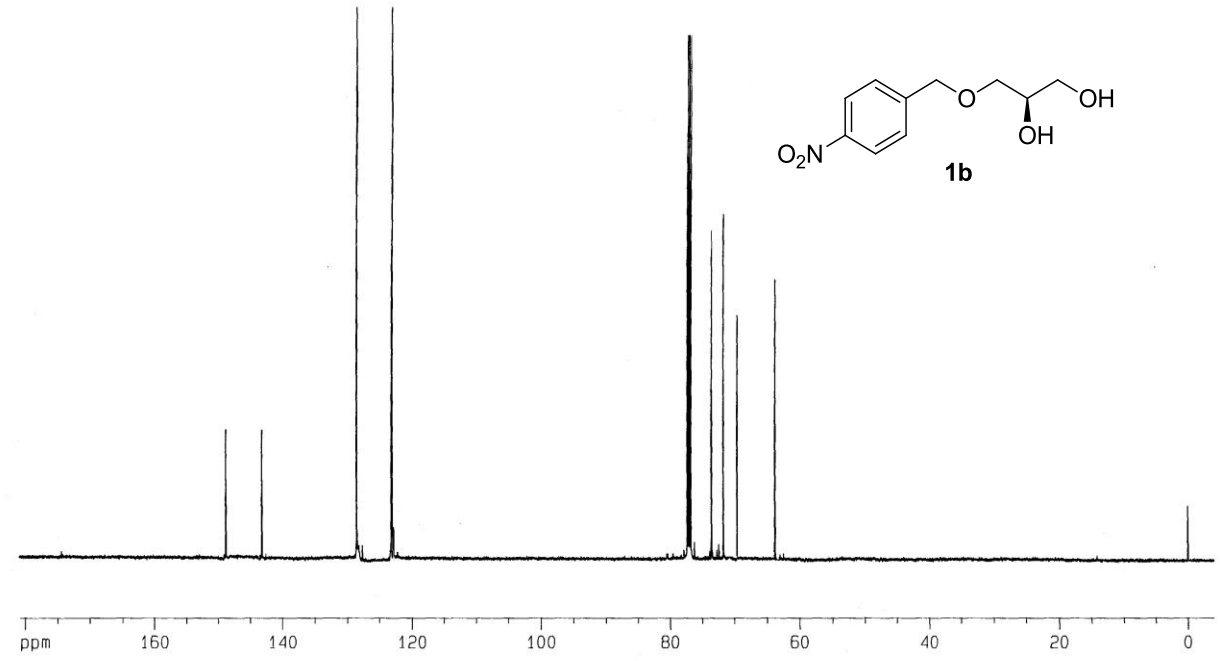


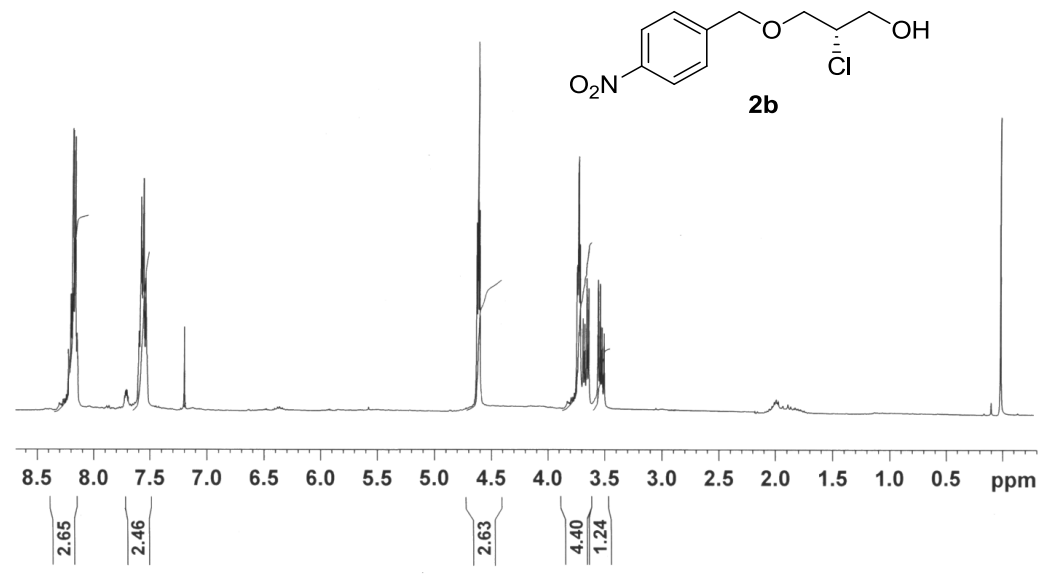


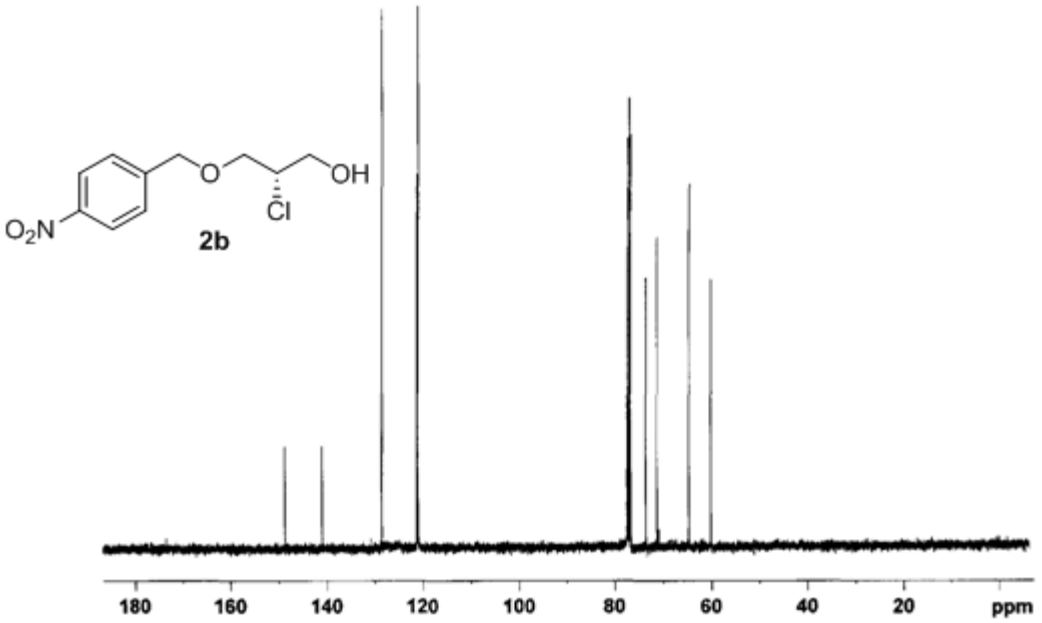
(*S*)-**23**

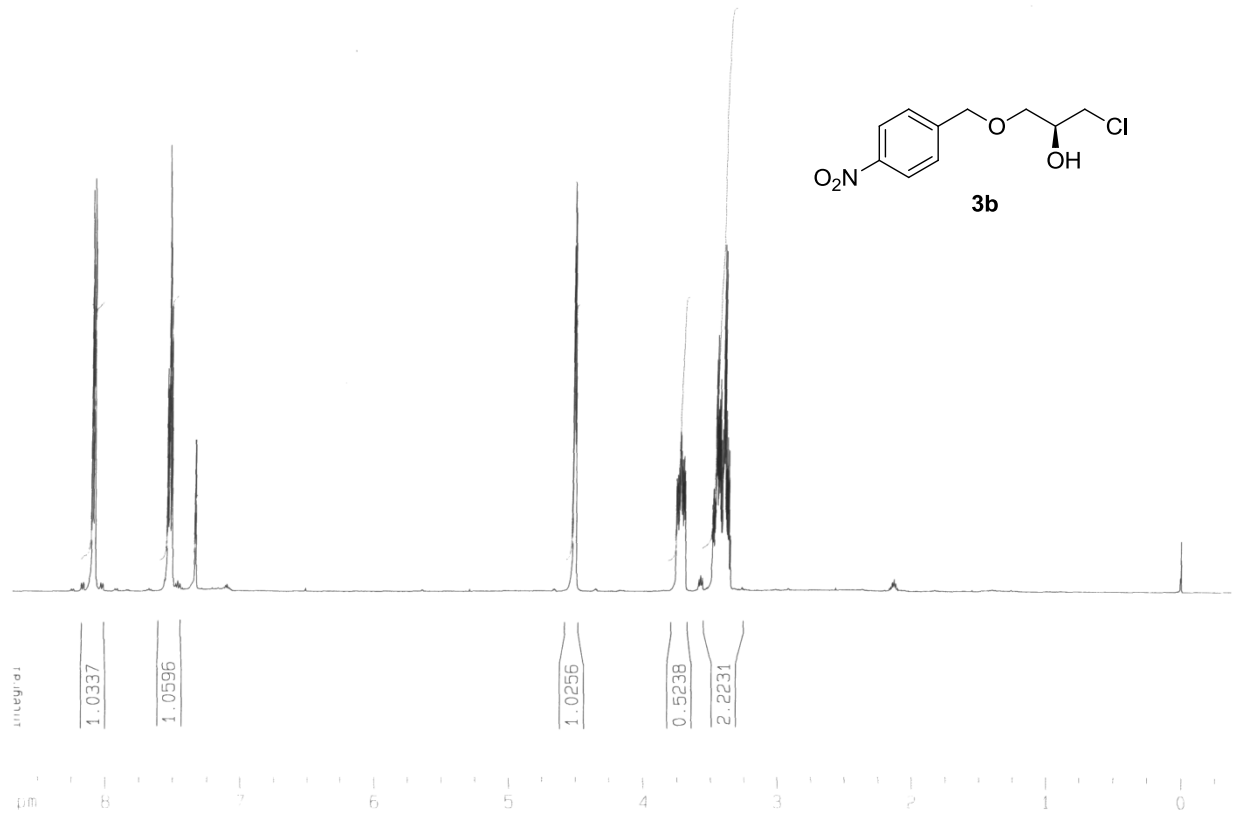


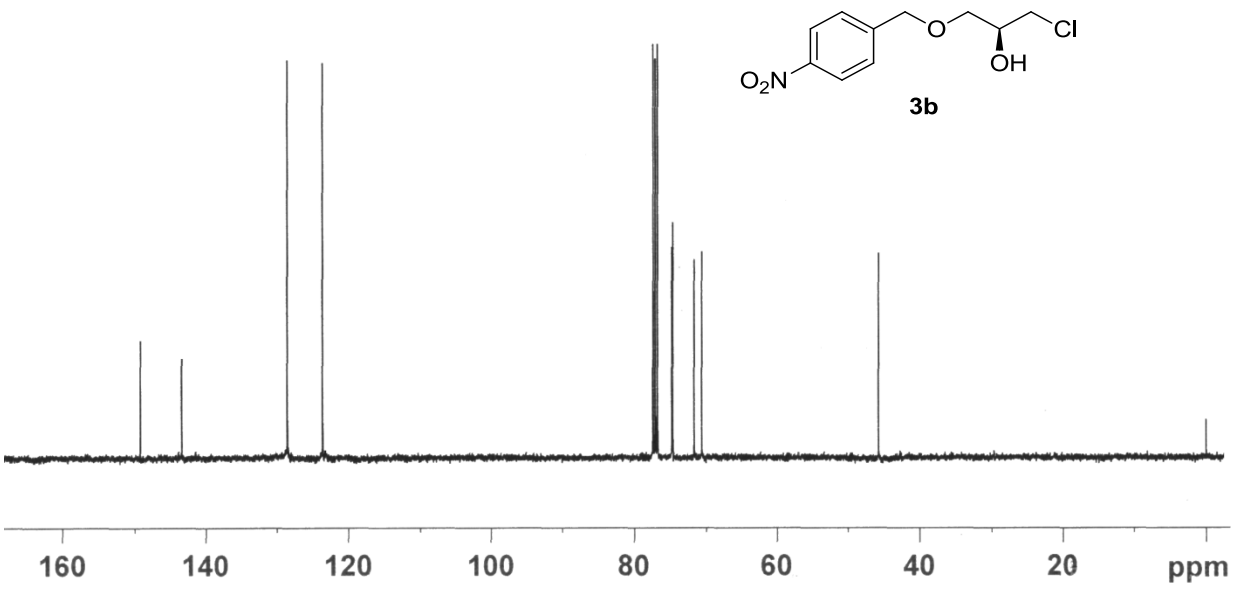


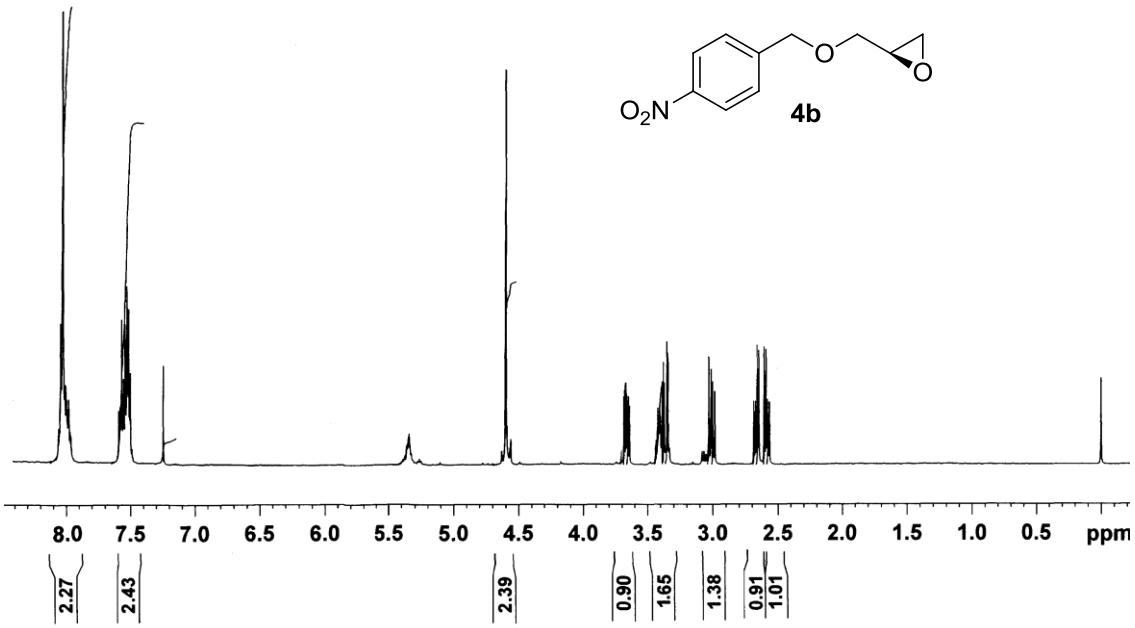


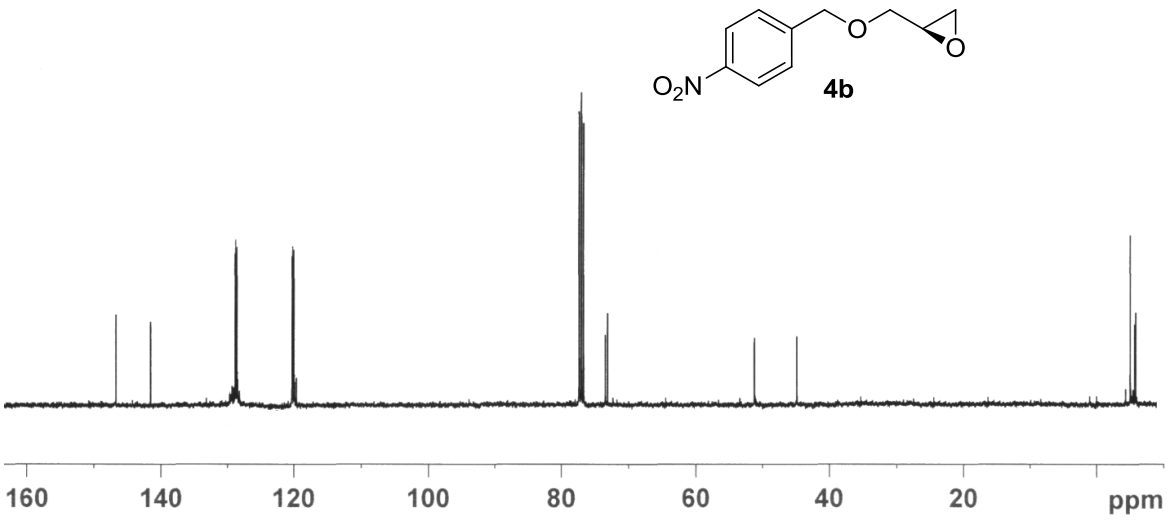


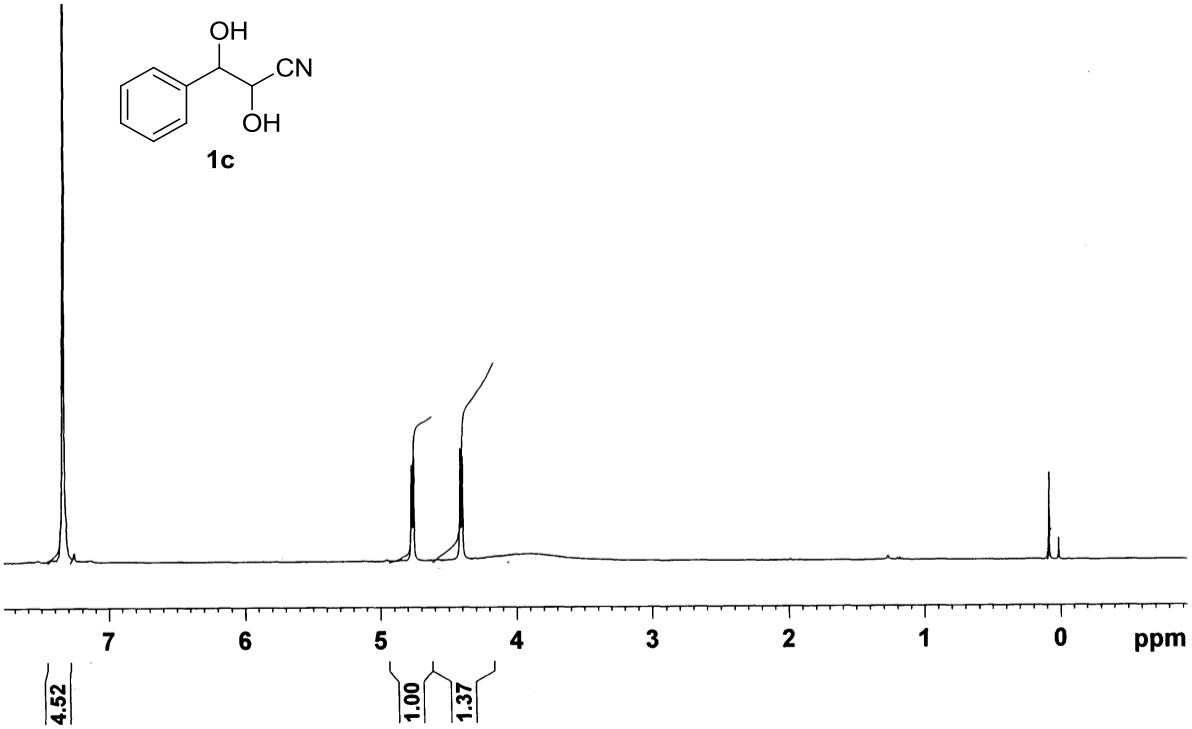


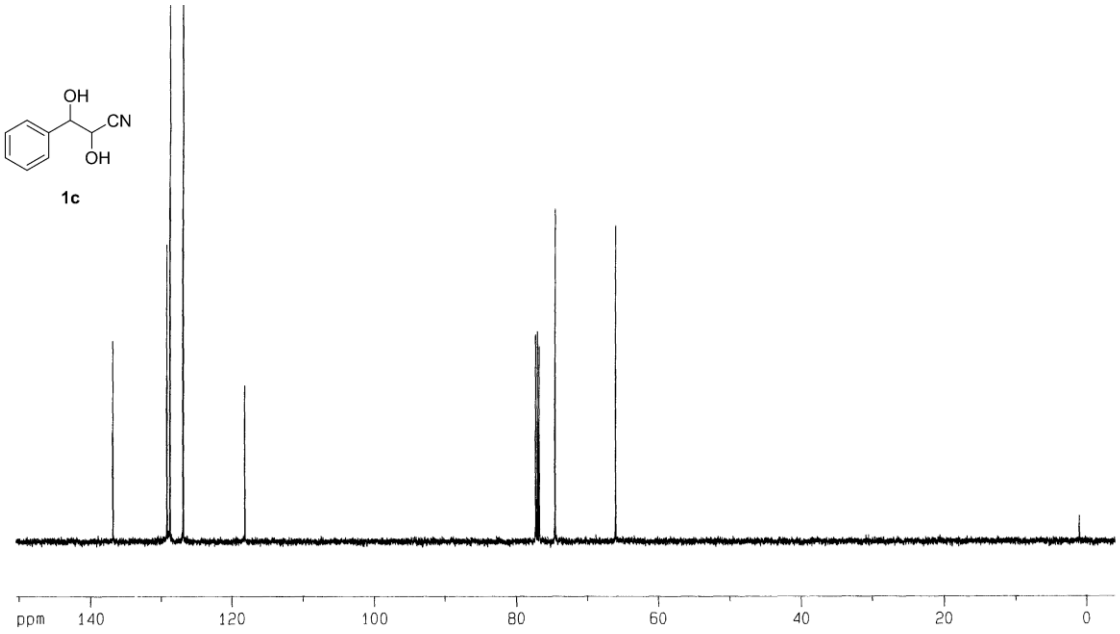


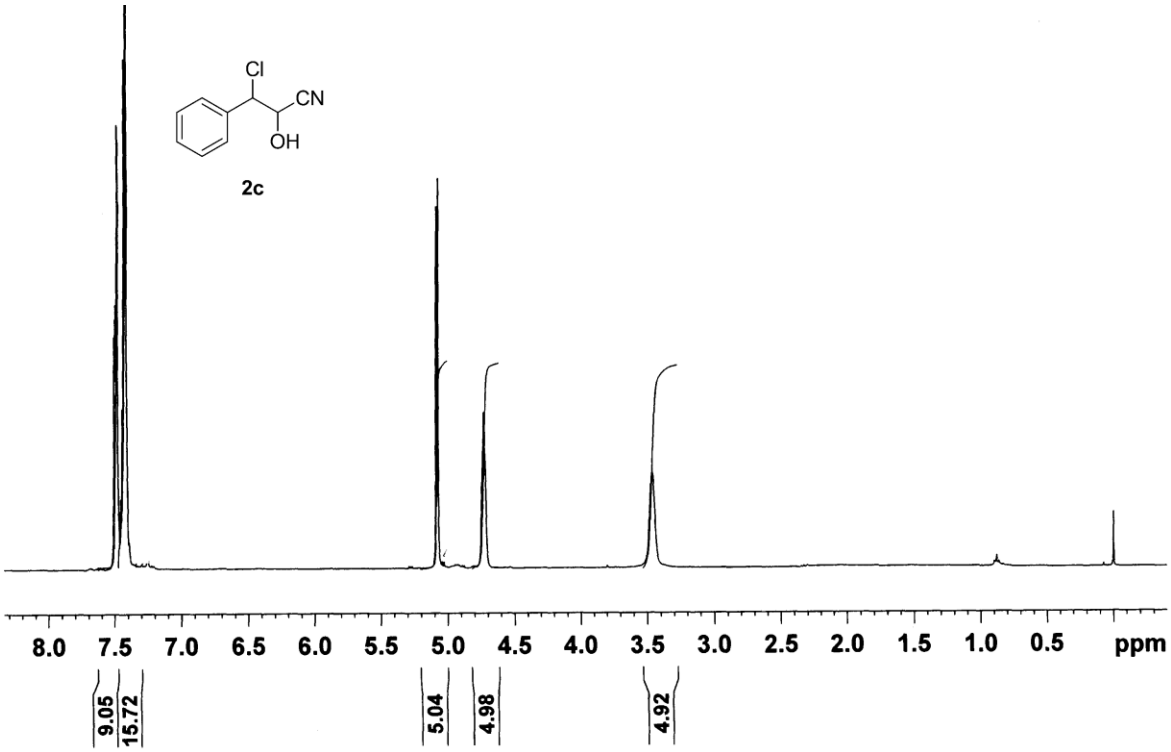


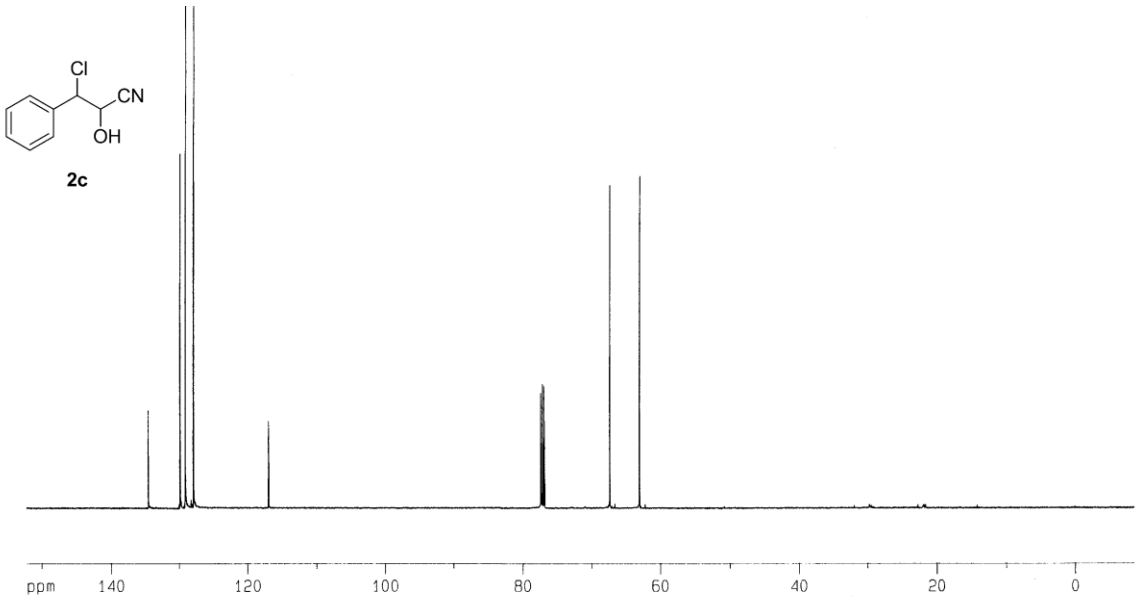


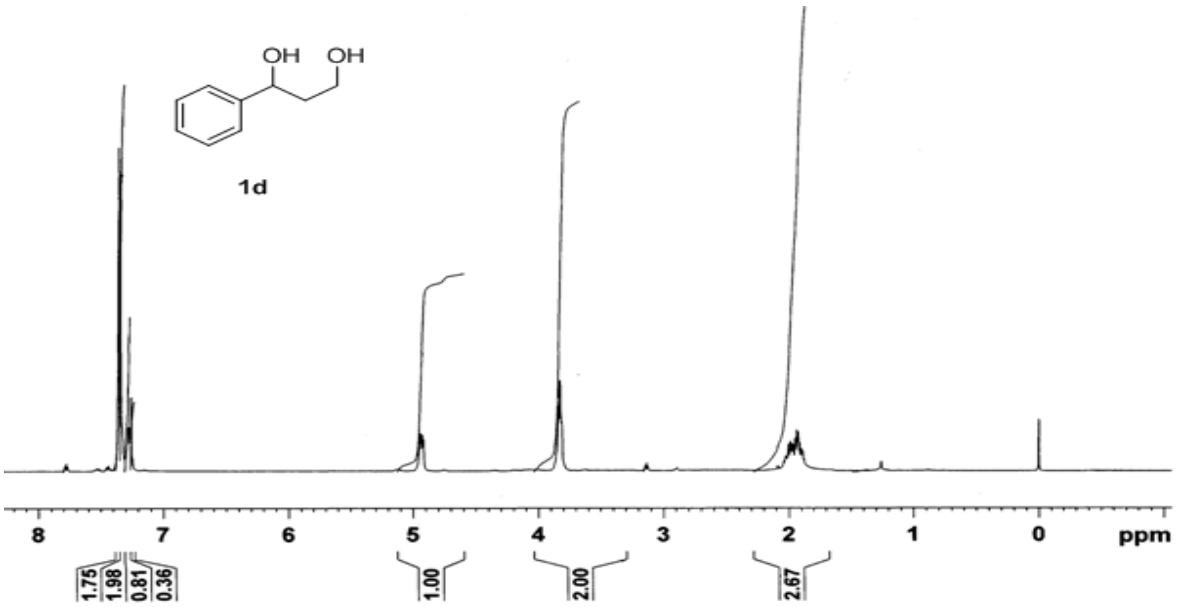


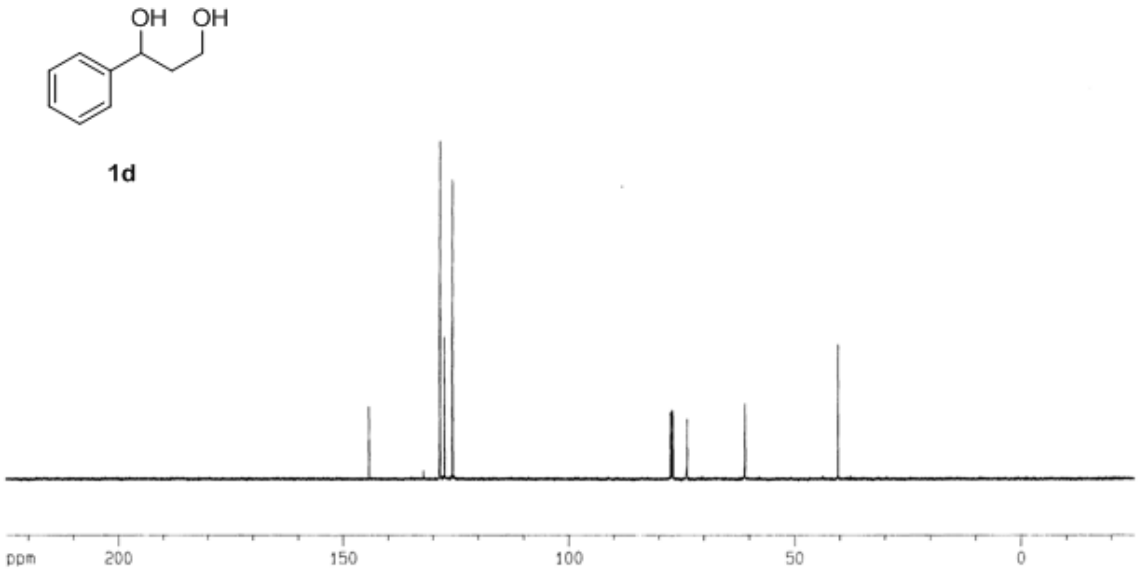


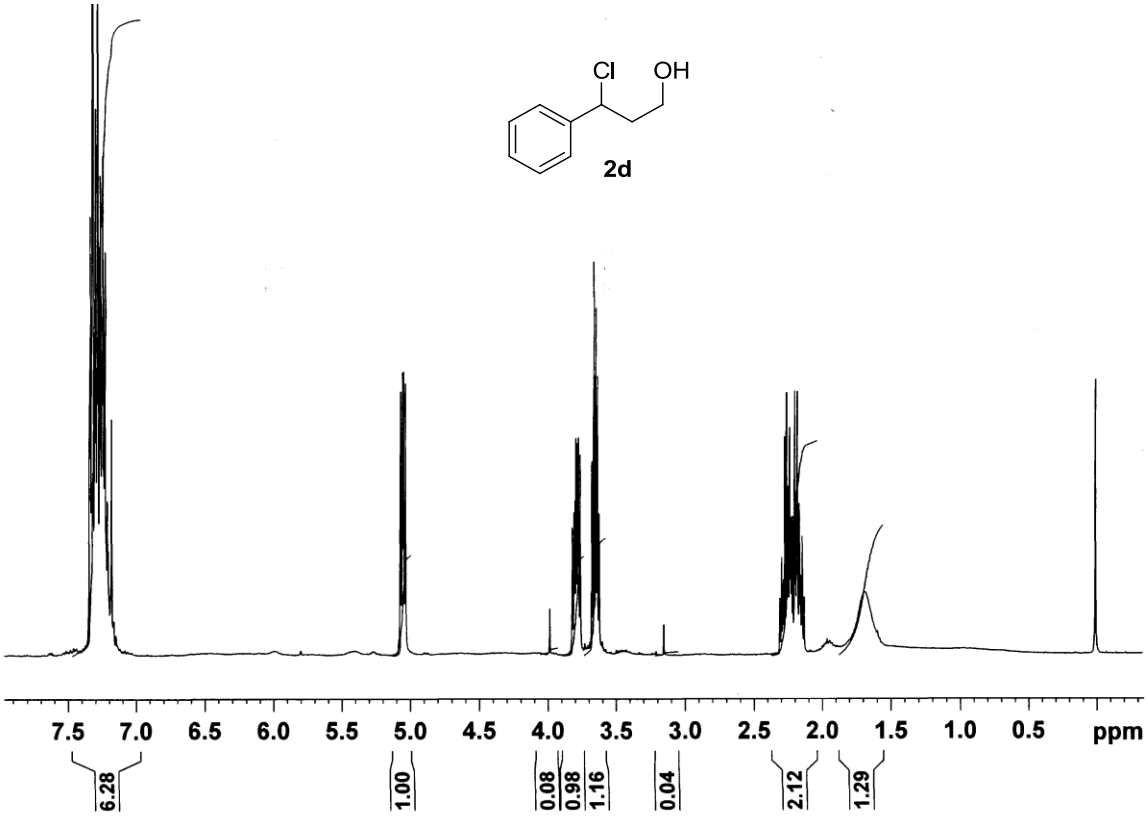


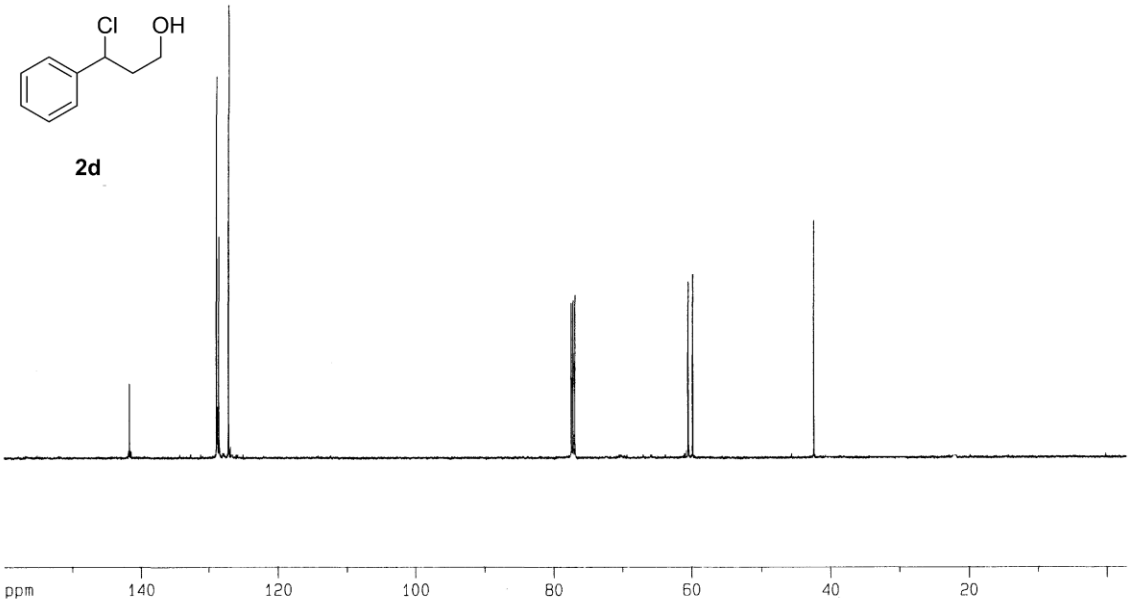


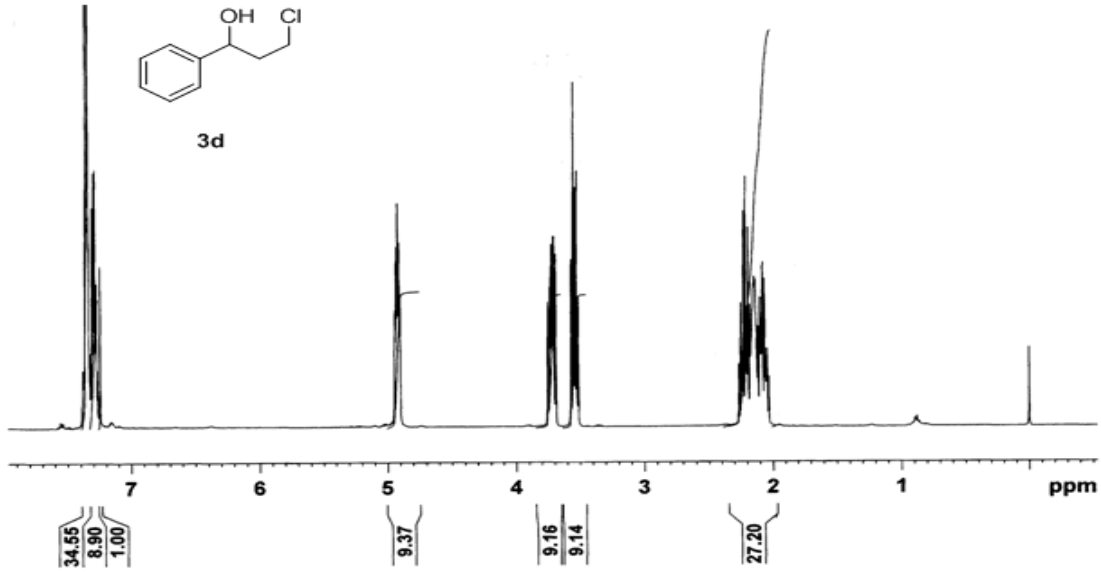


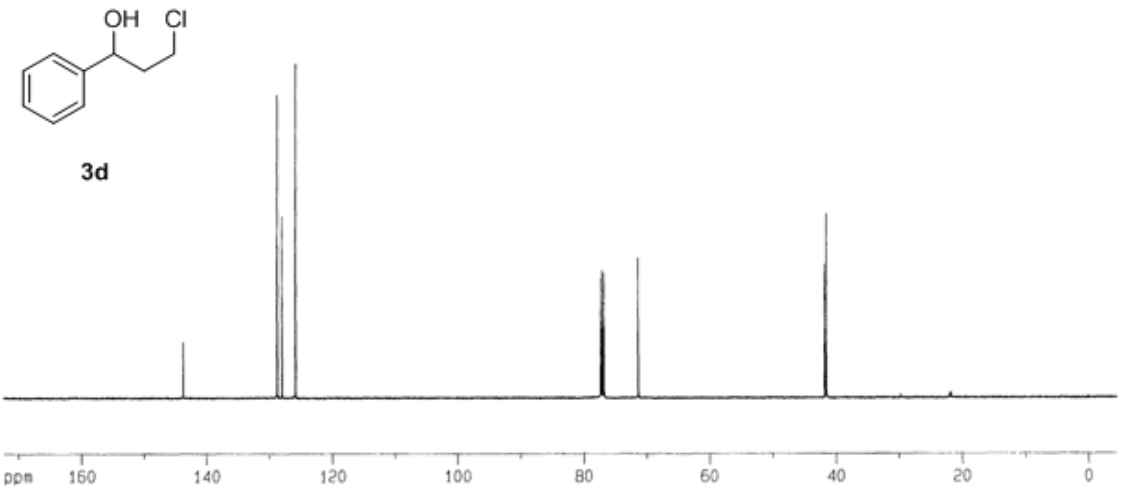


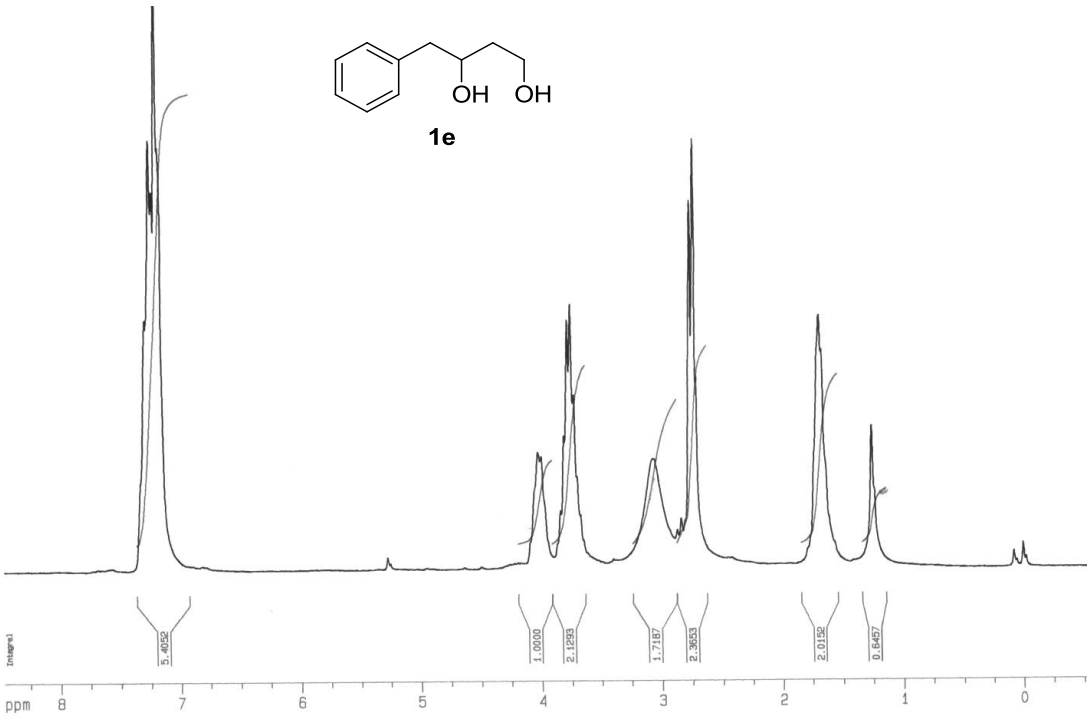


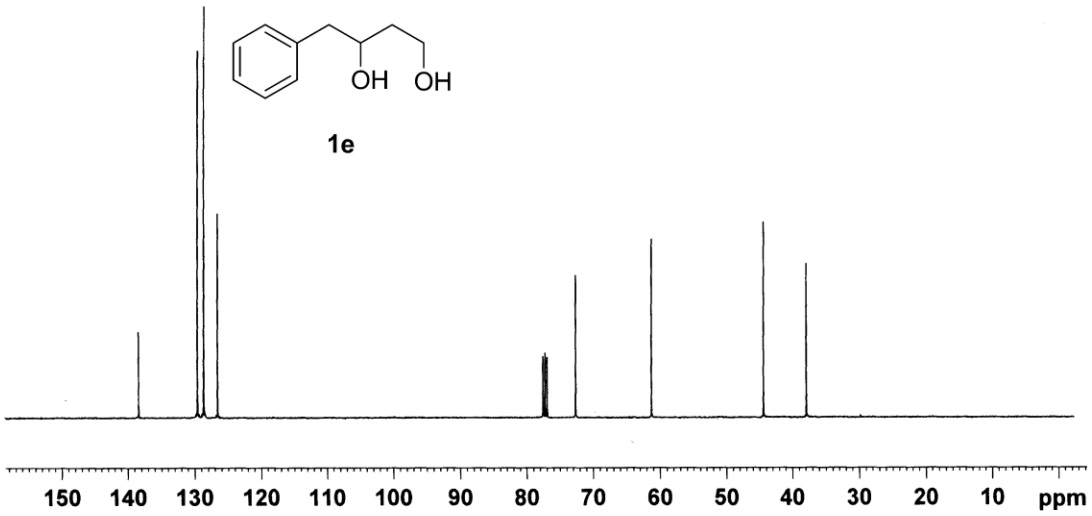


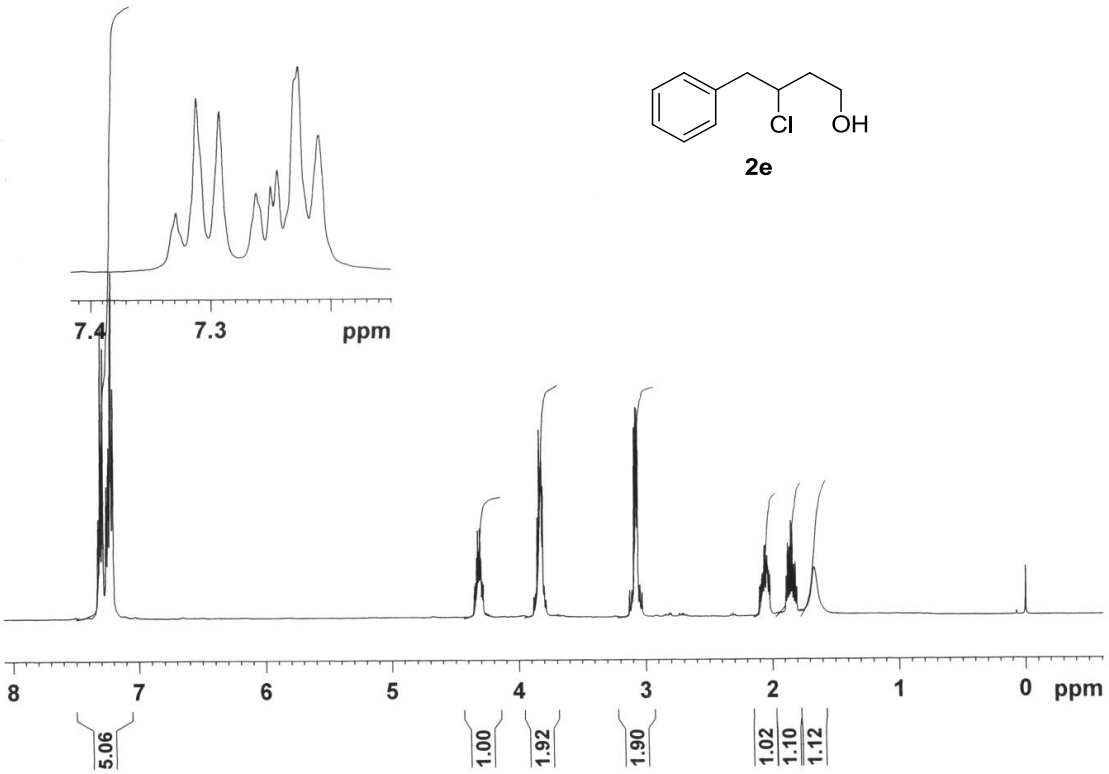


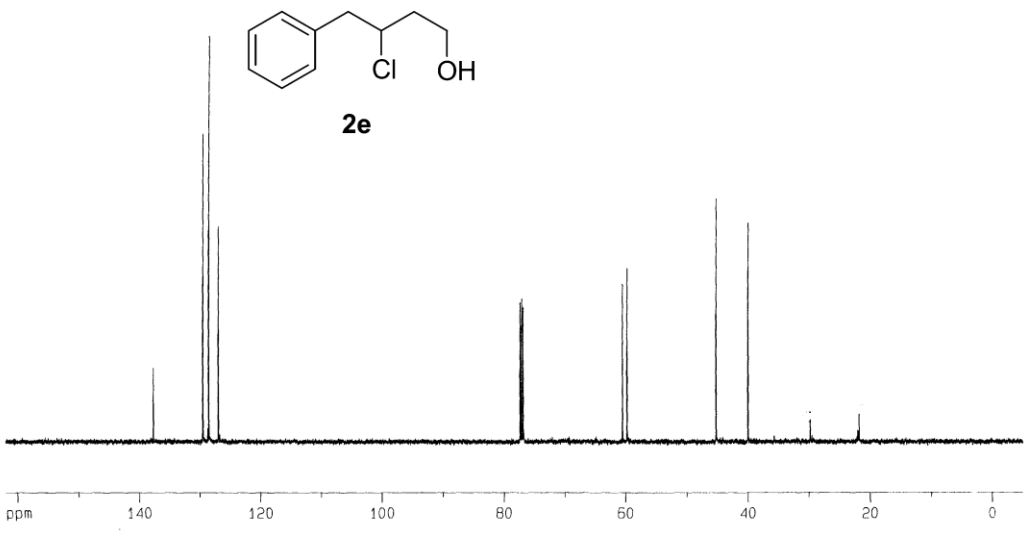


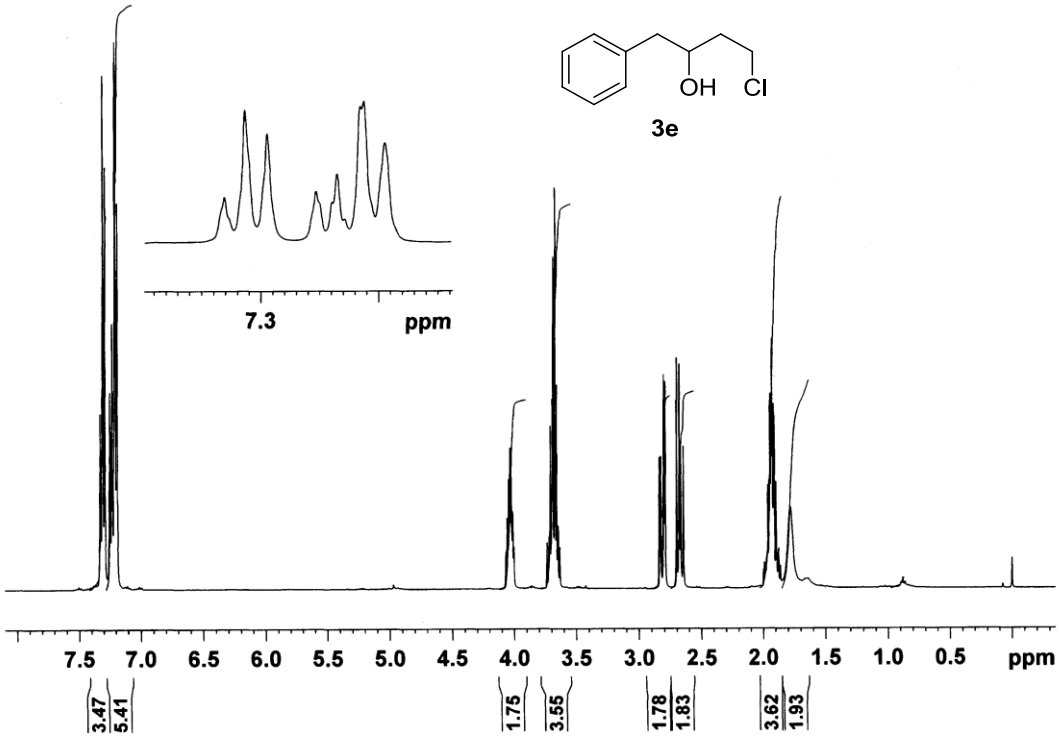


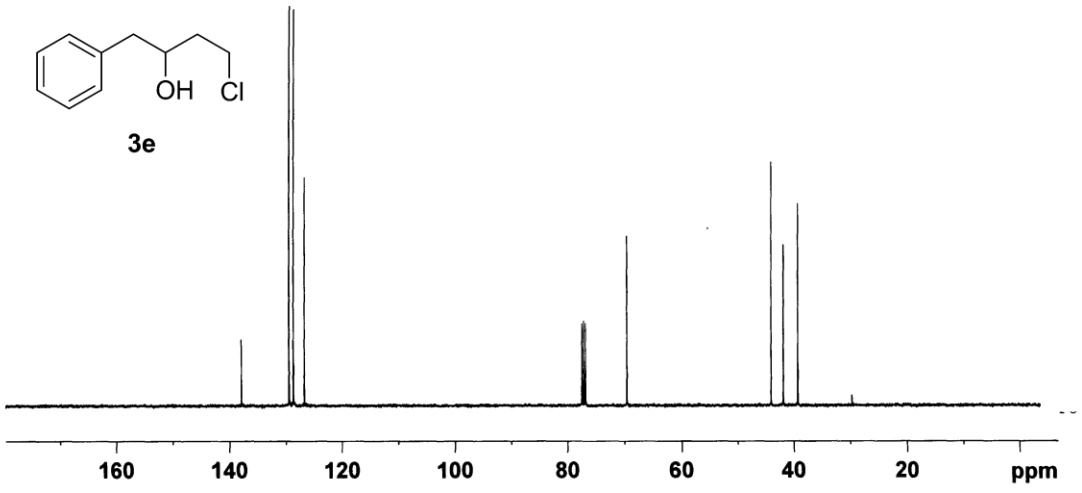


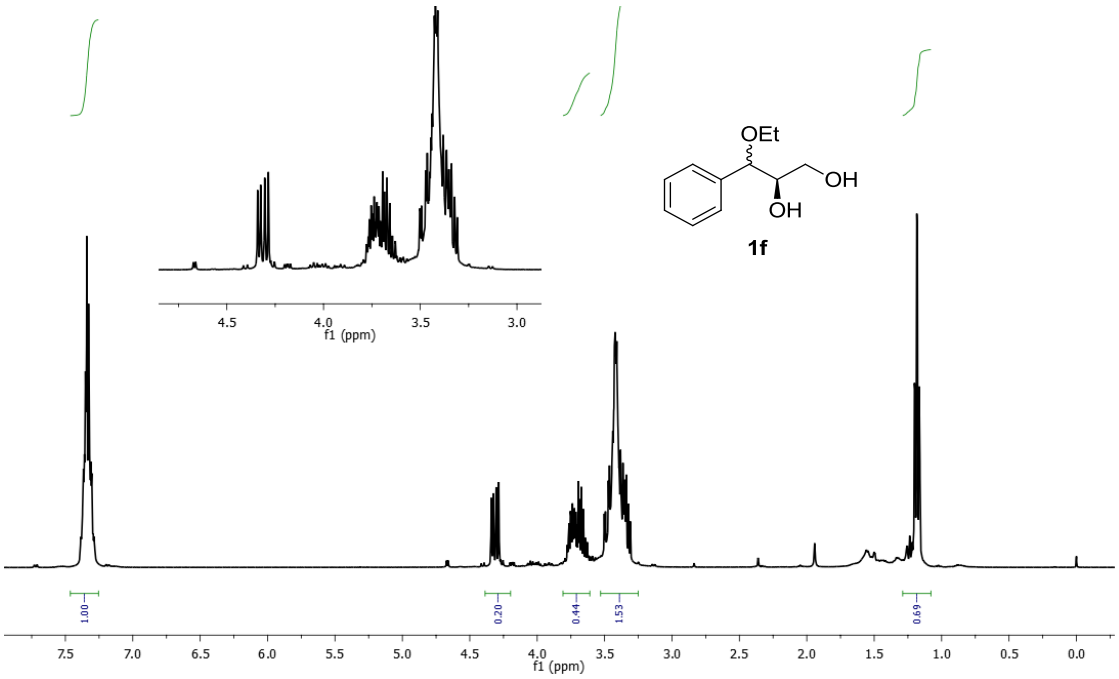


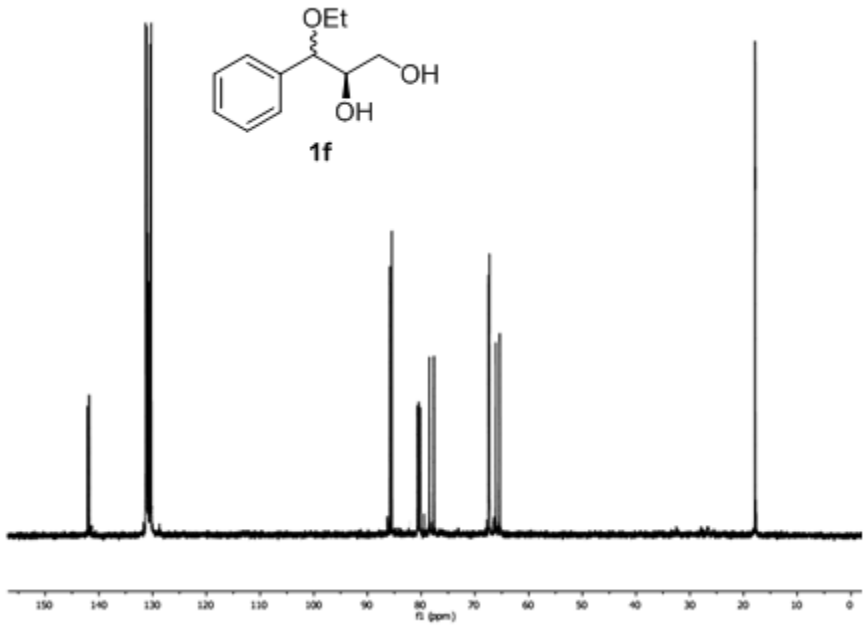


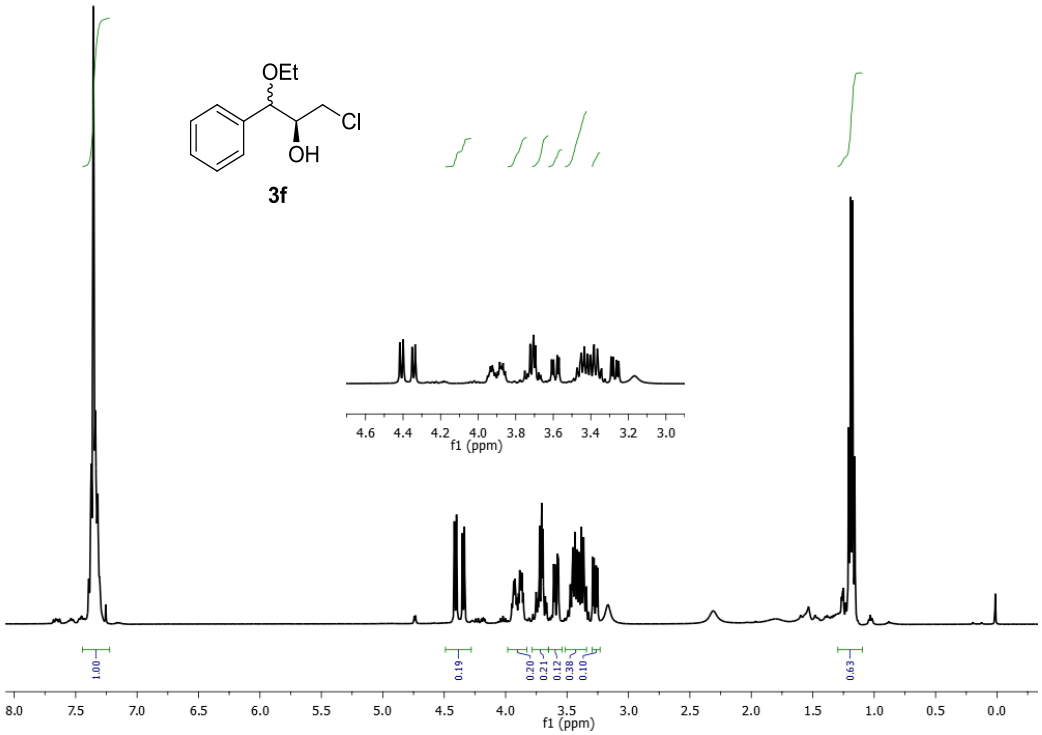


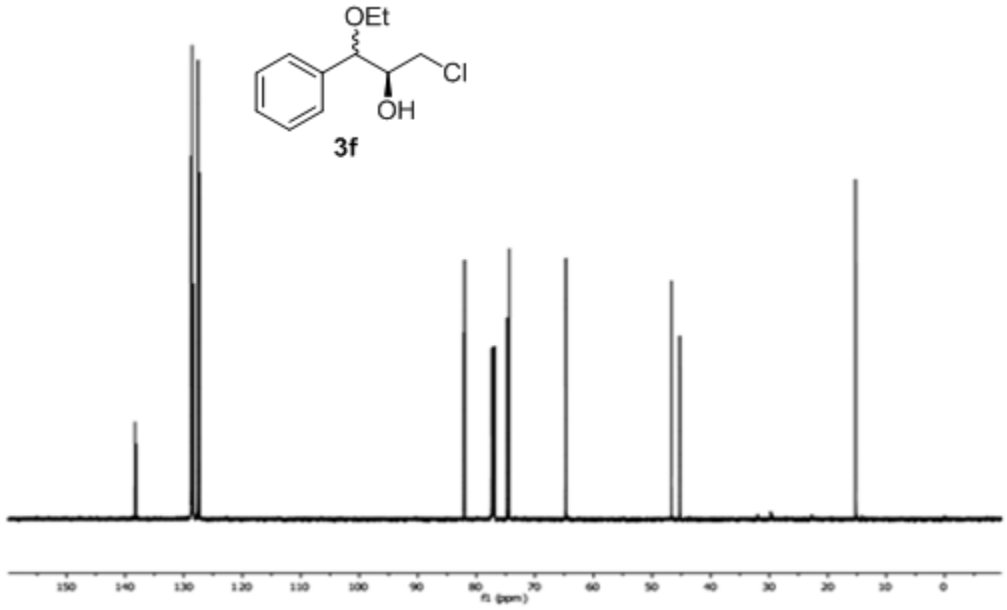


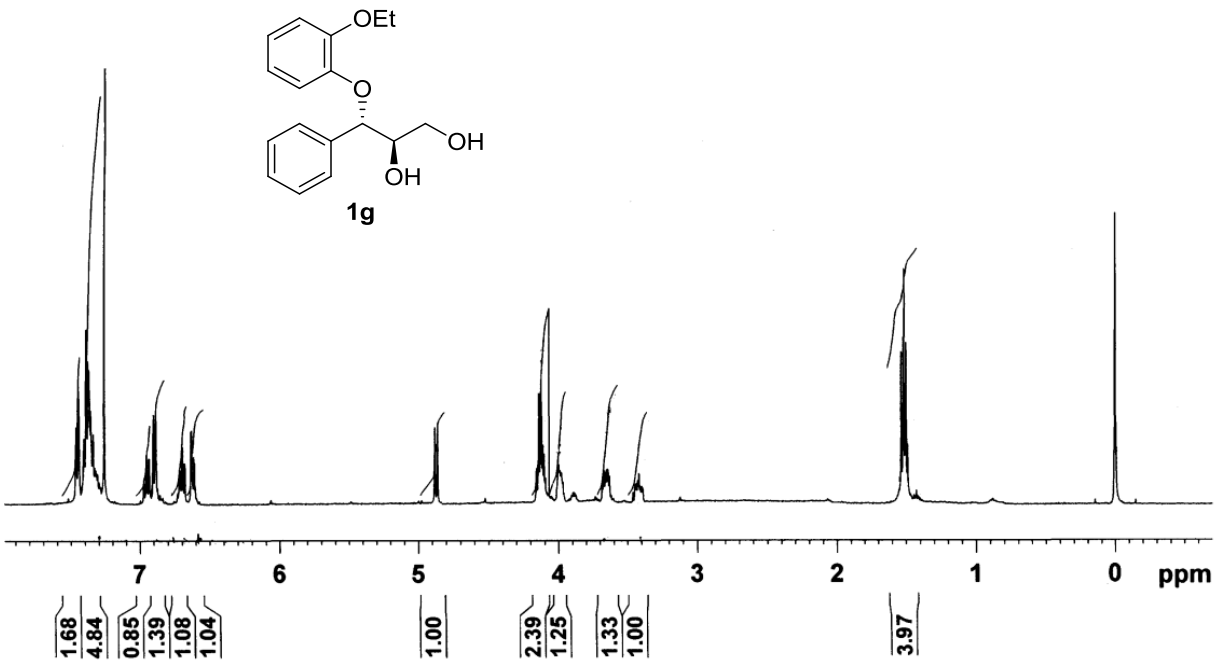


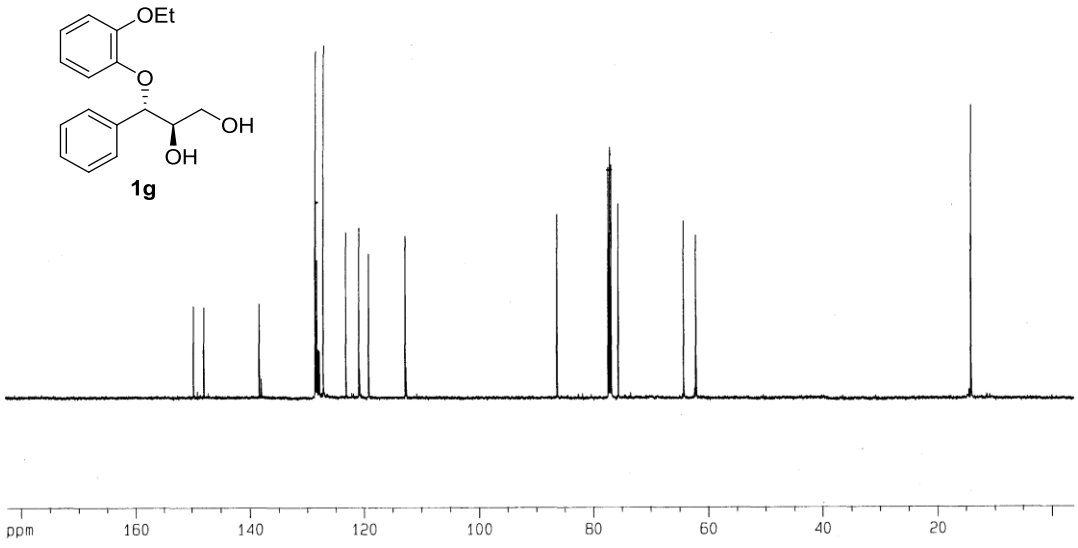


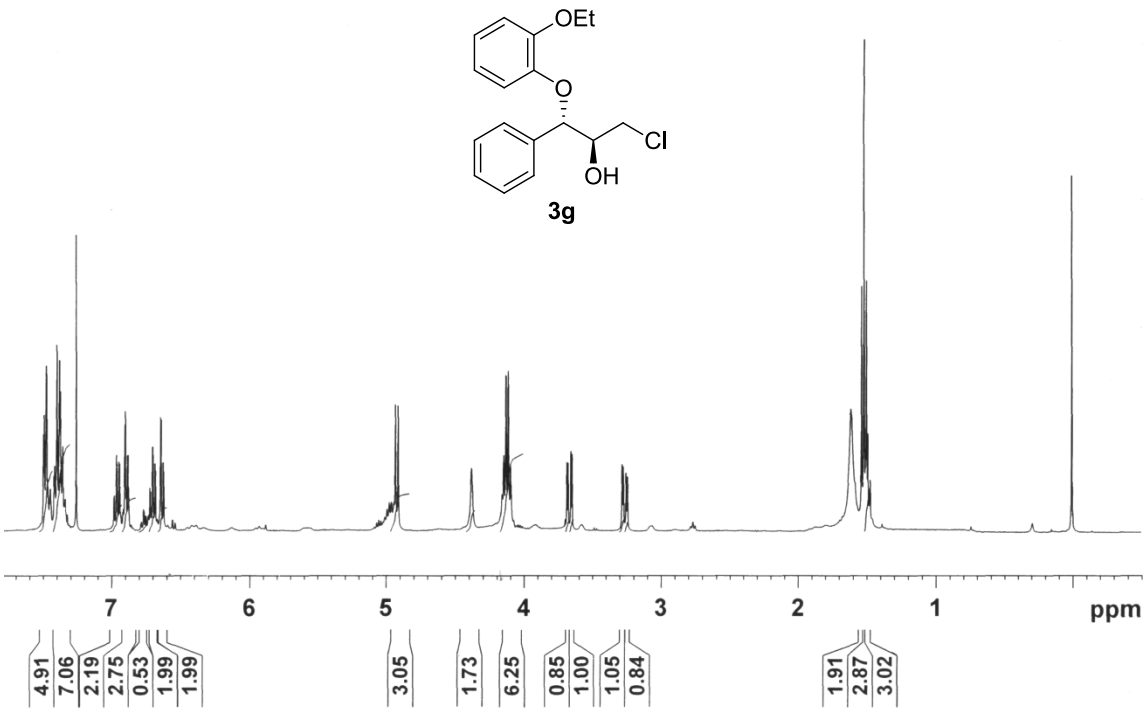


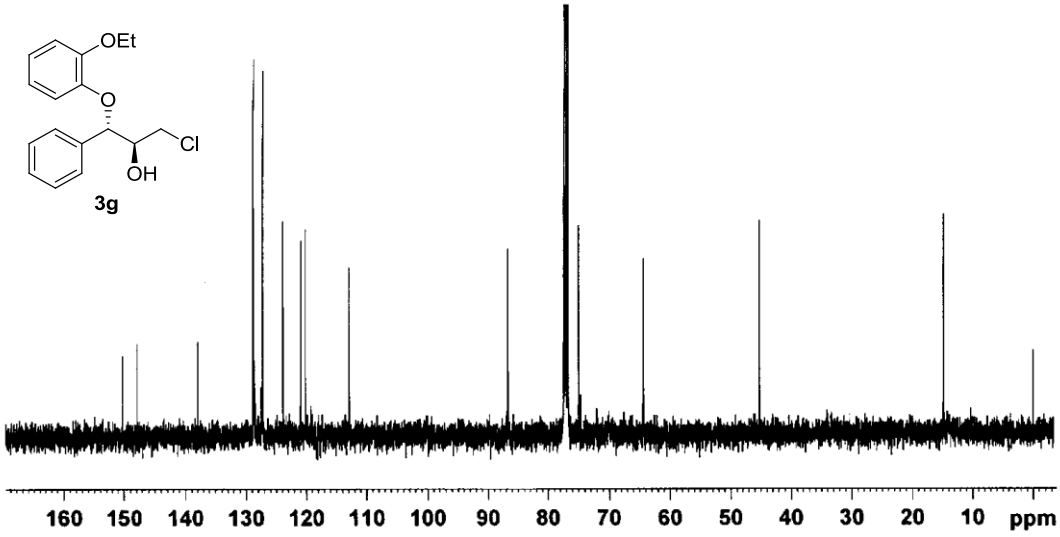


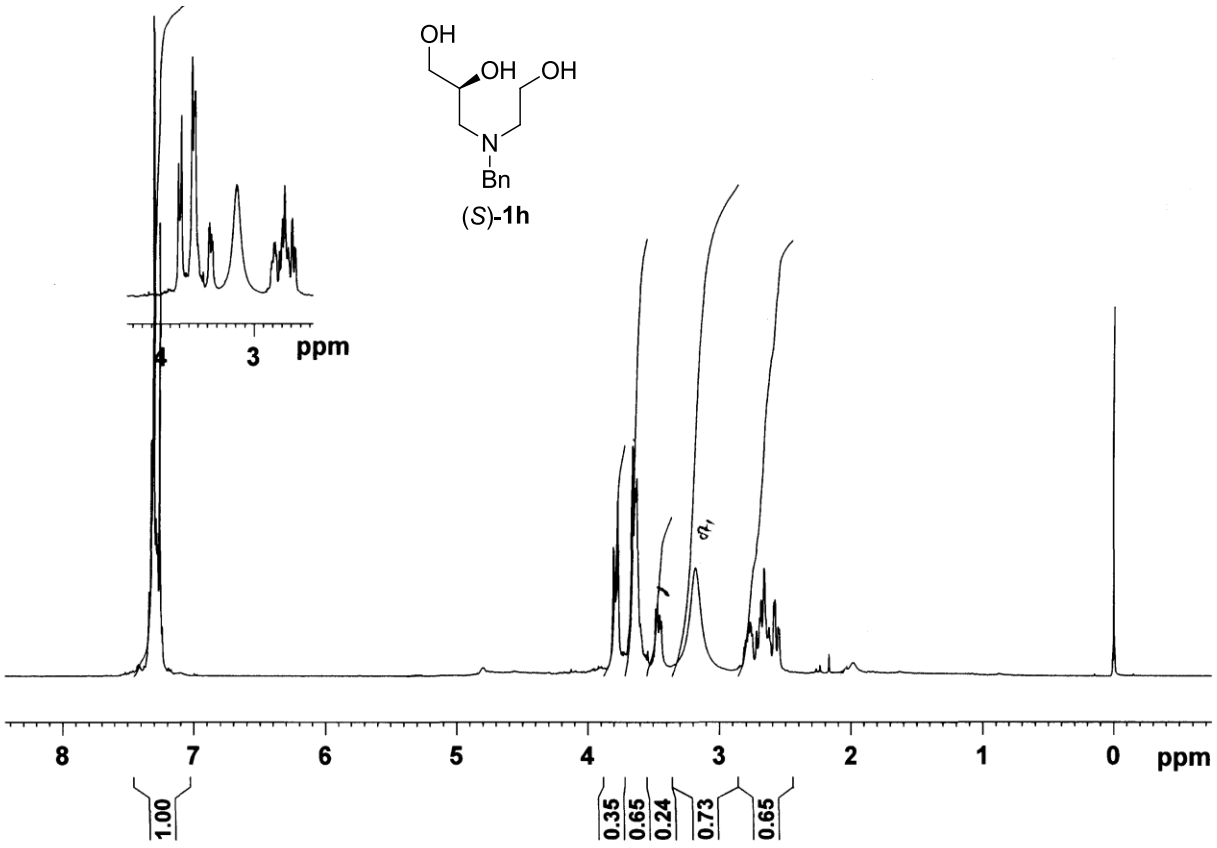


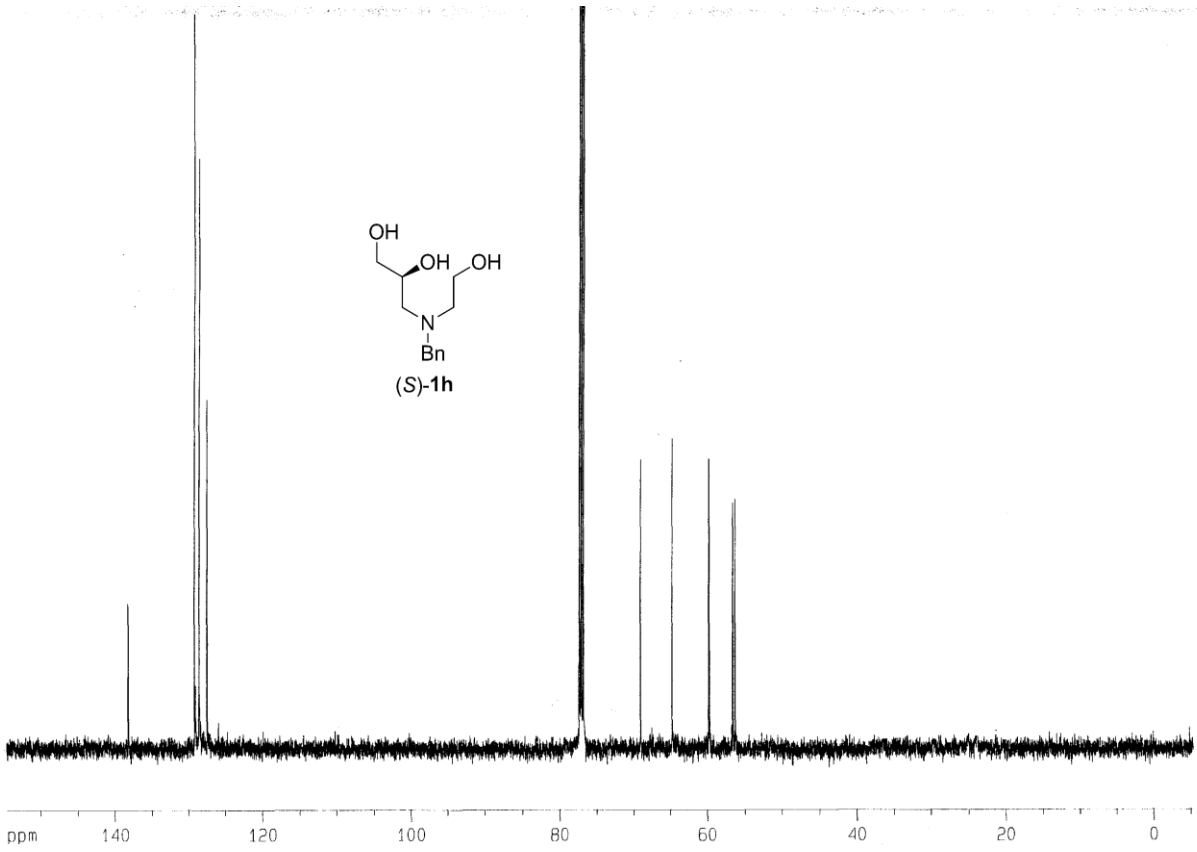


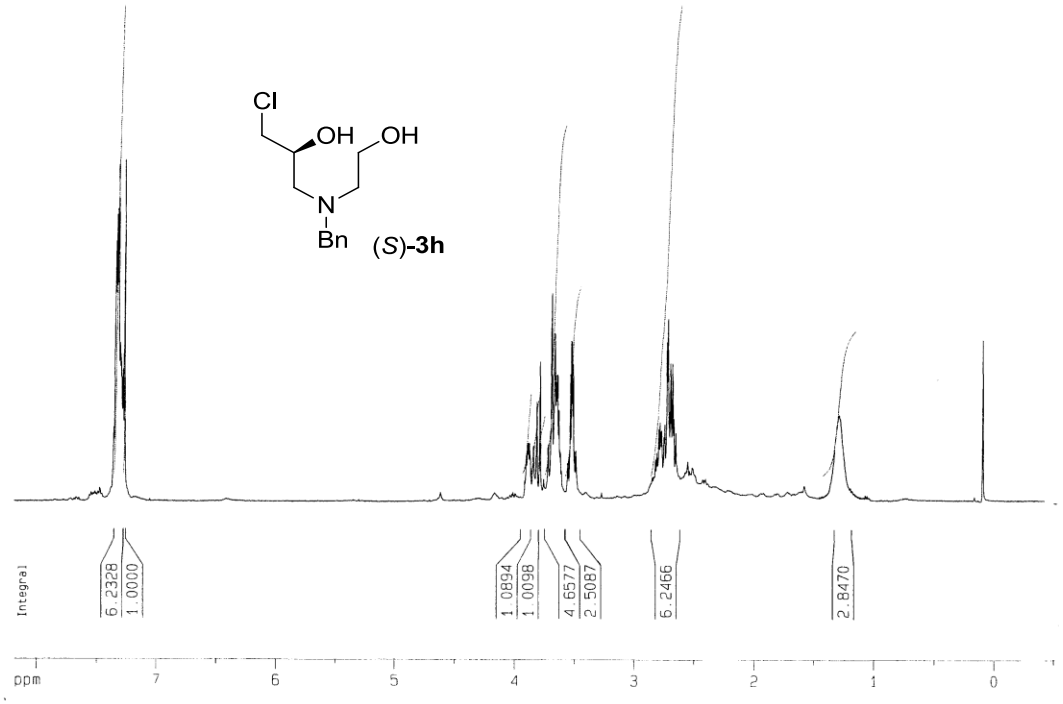


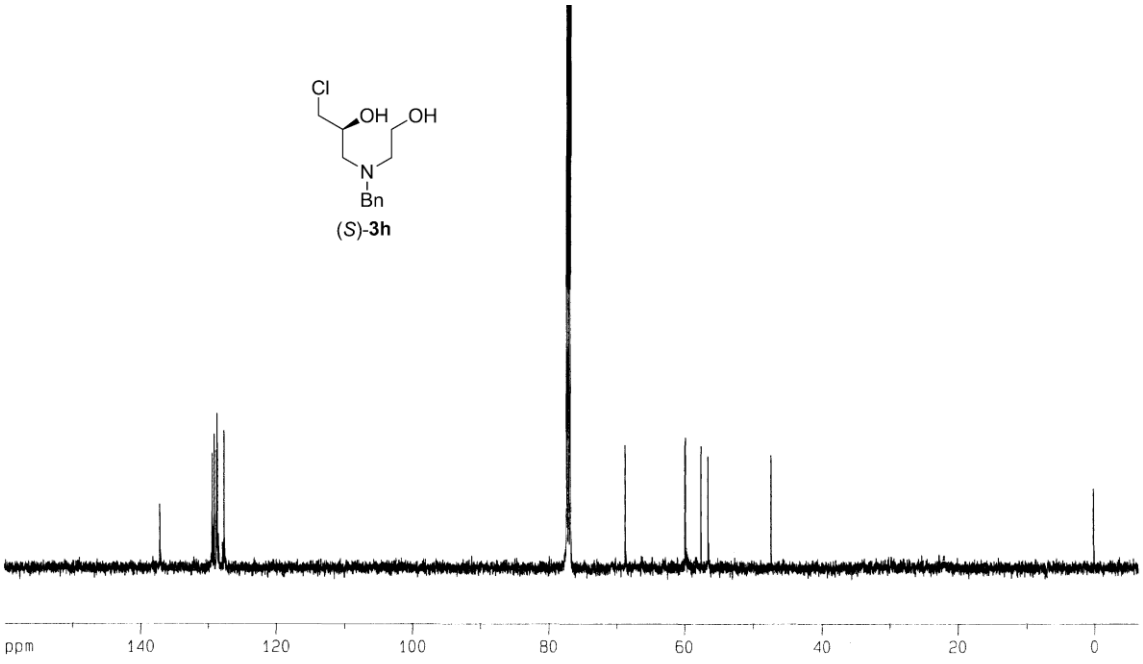


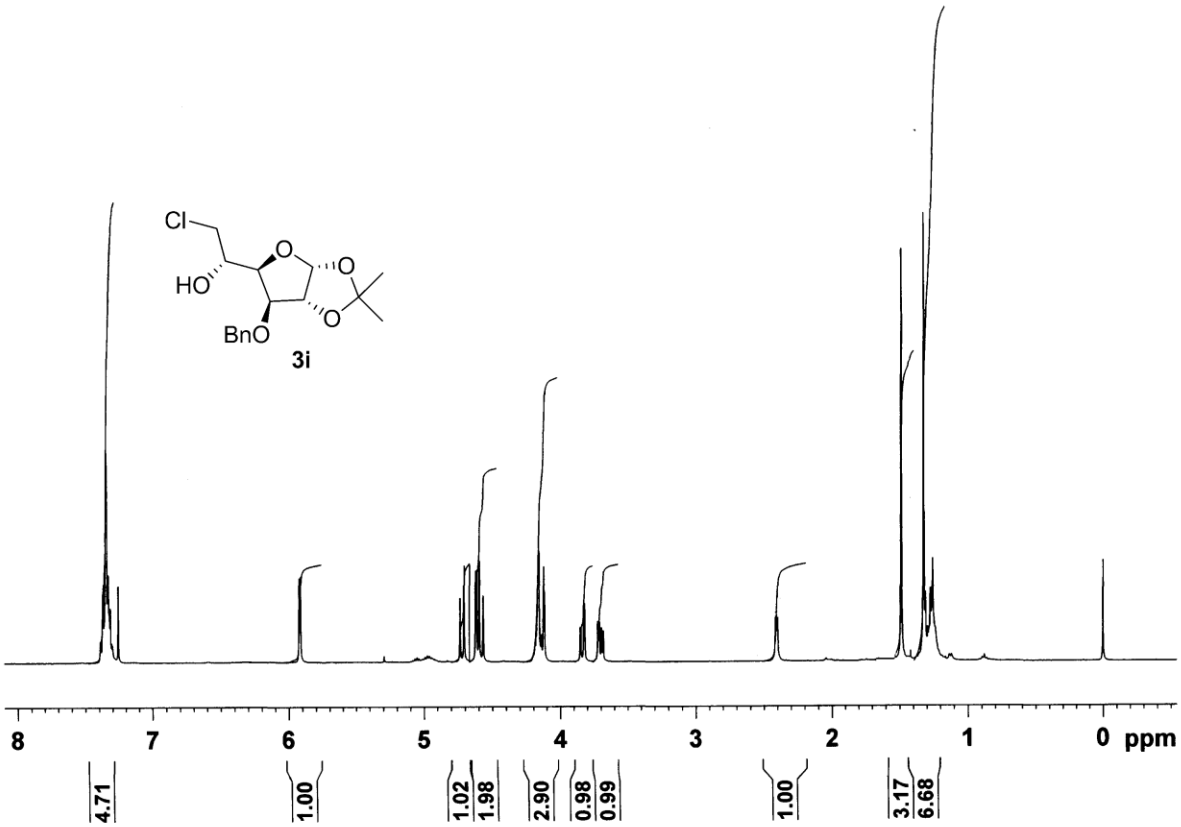


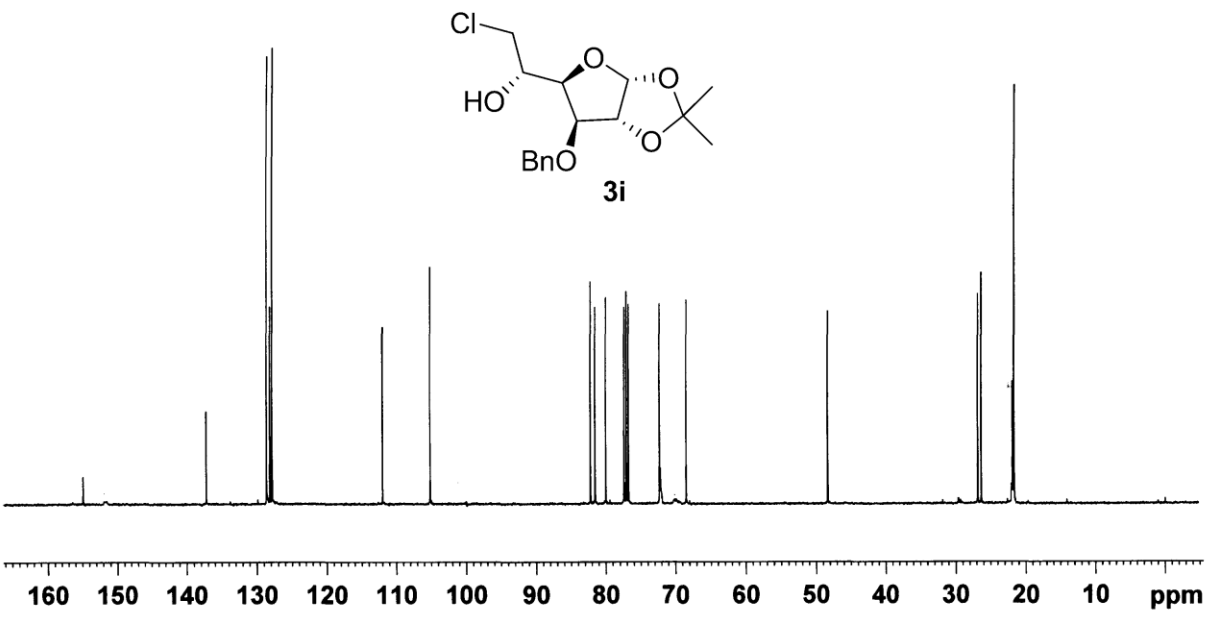


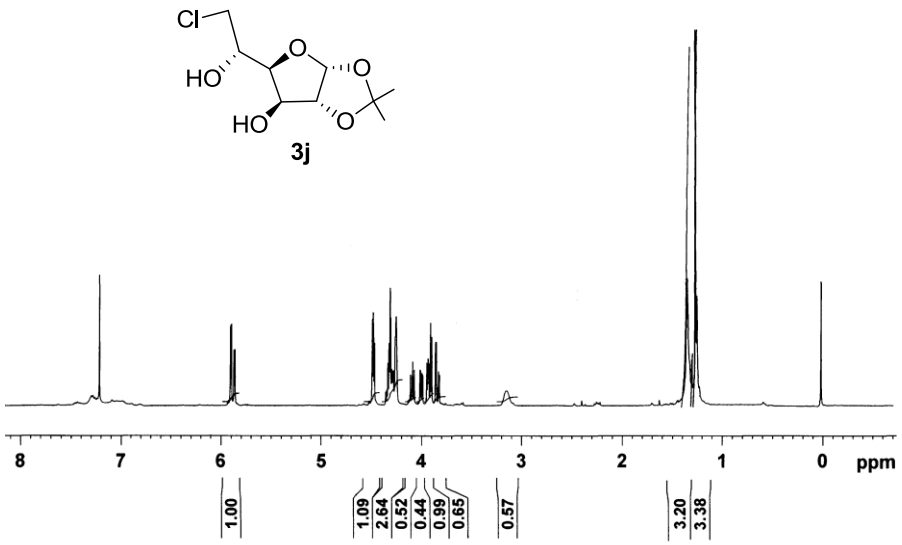


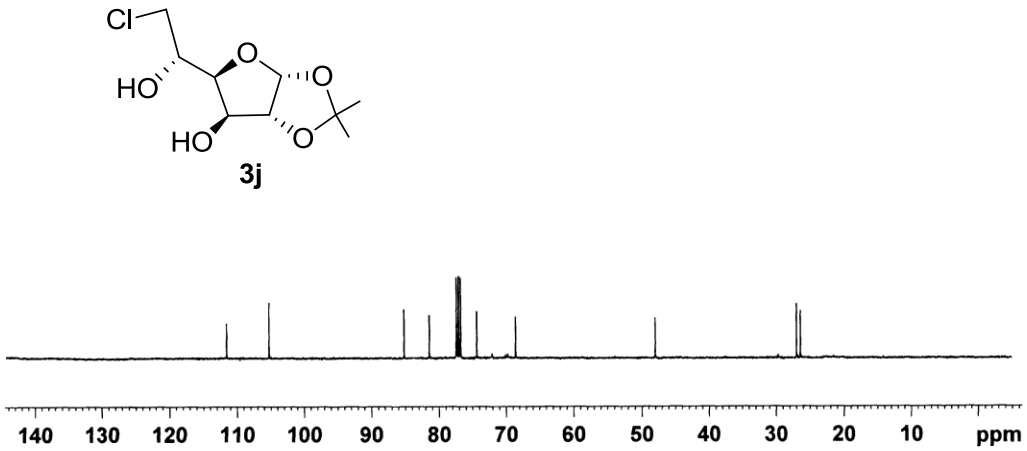


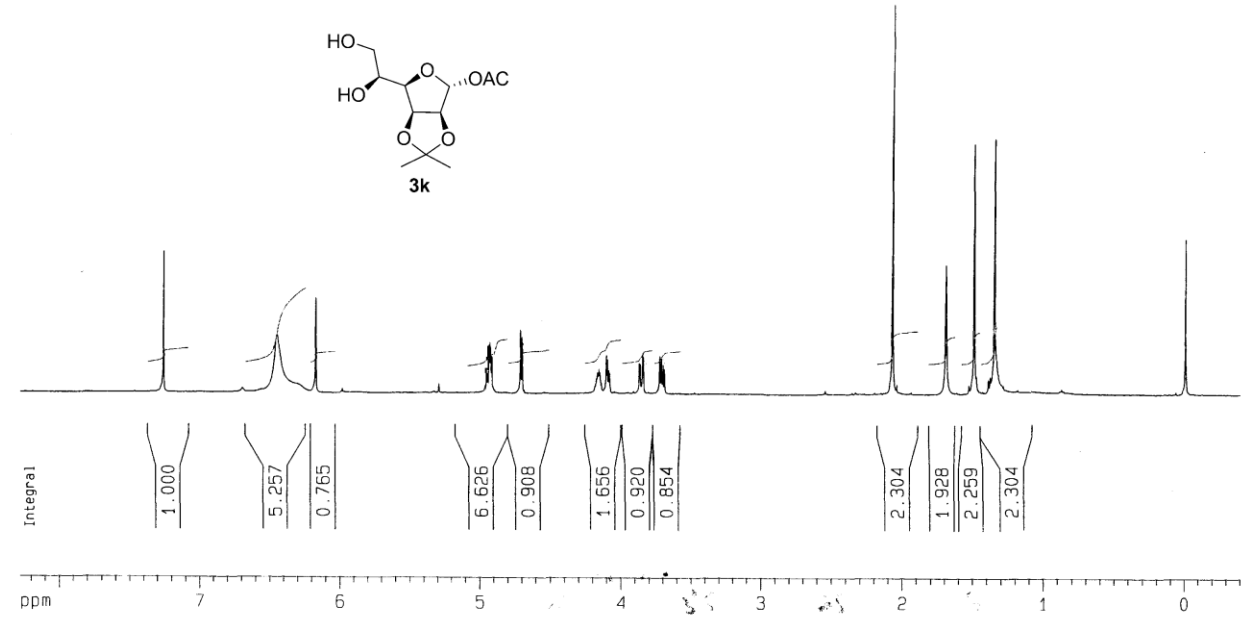


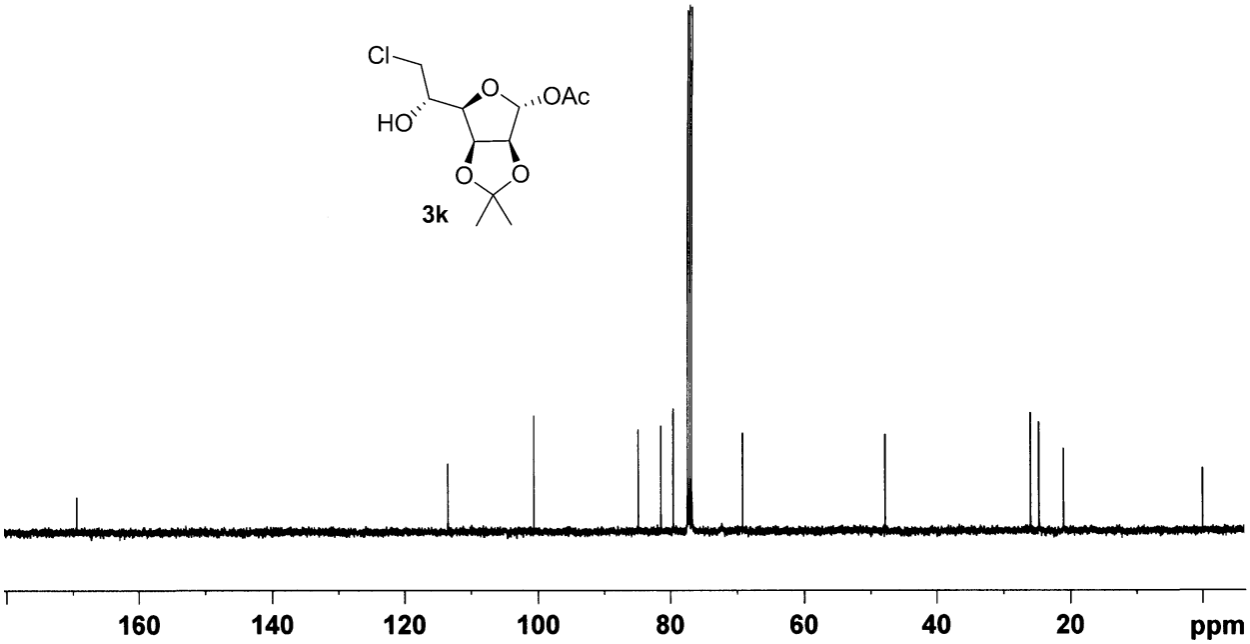


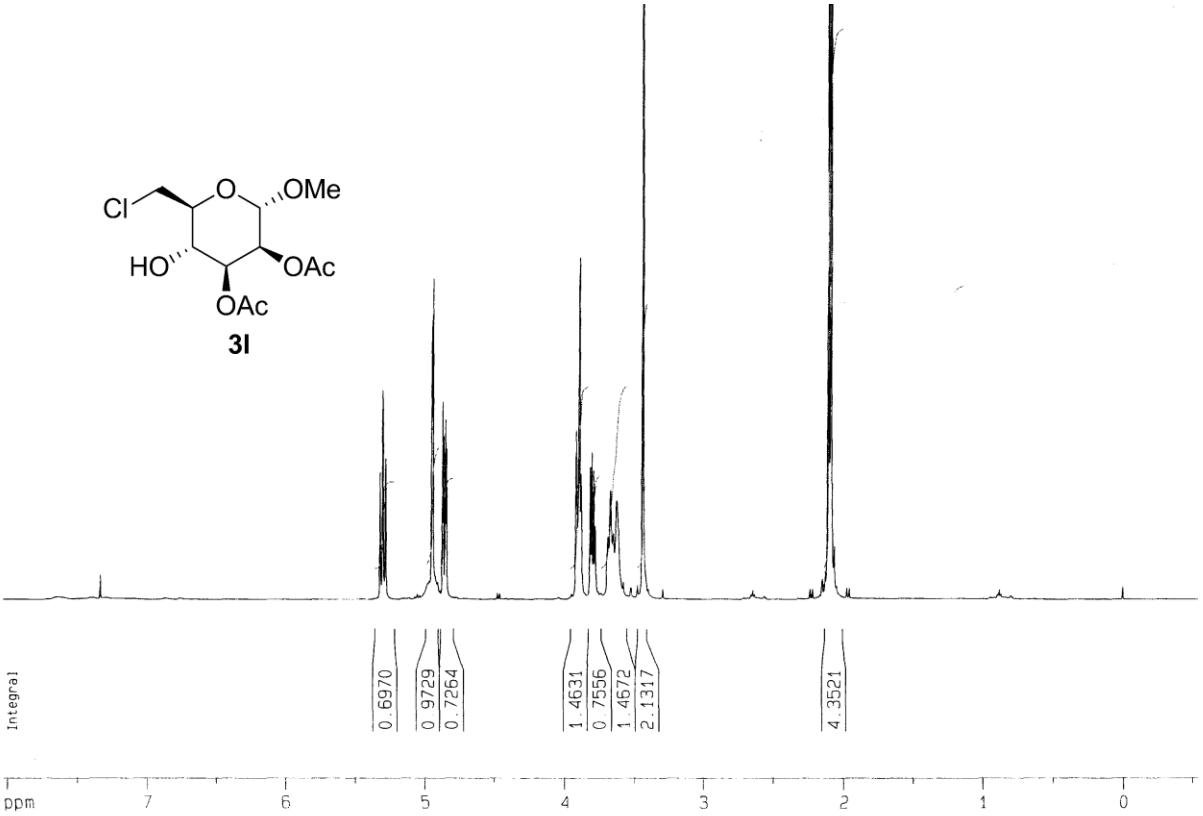


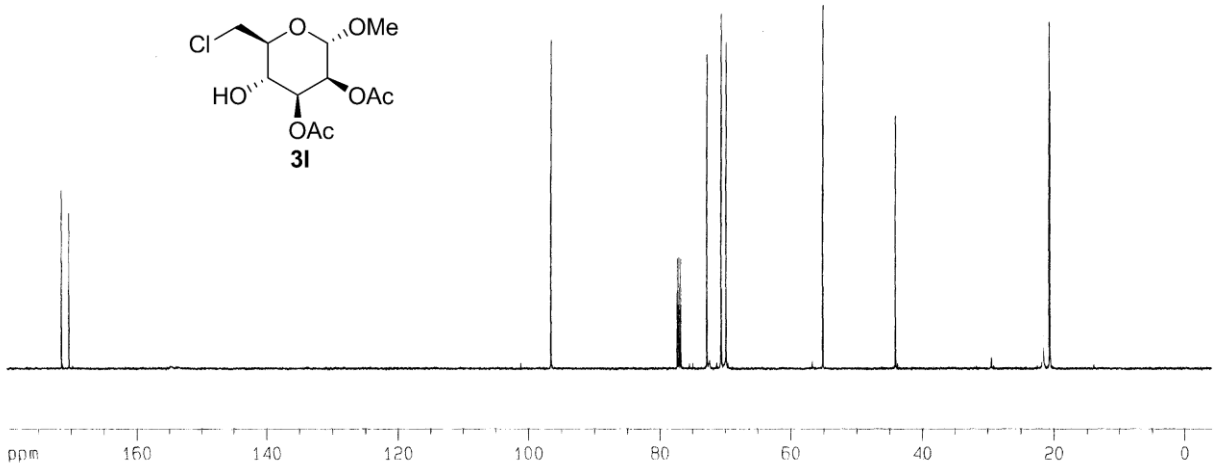


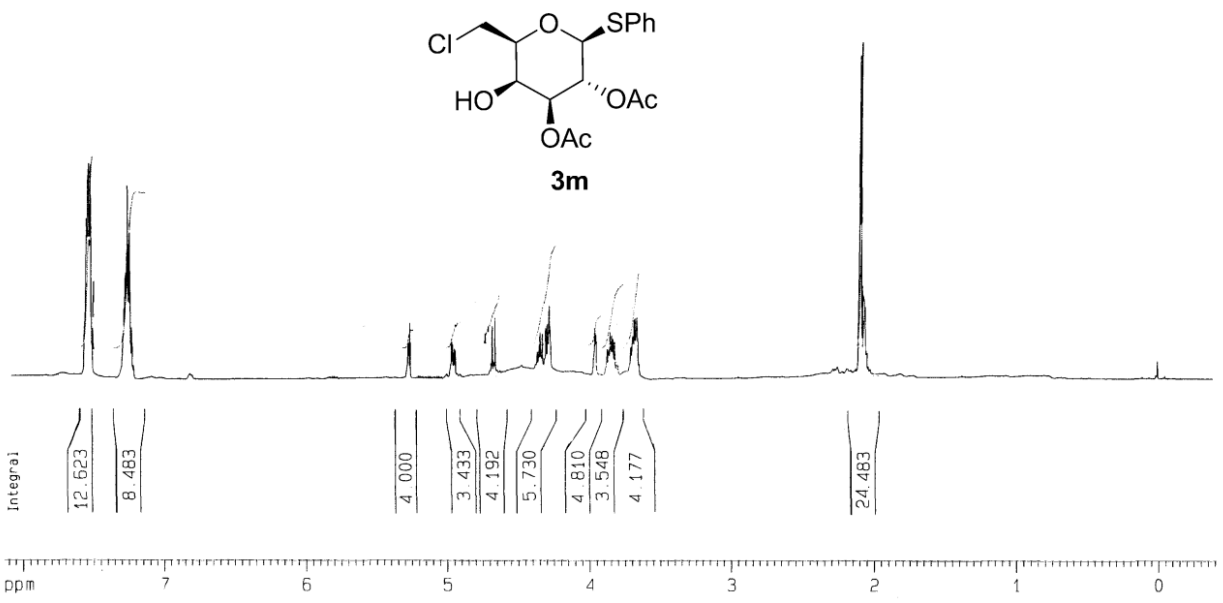


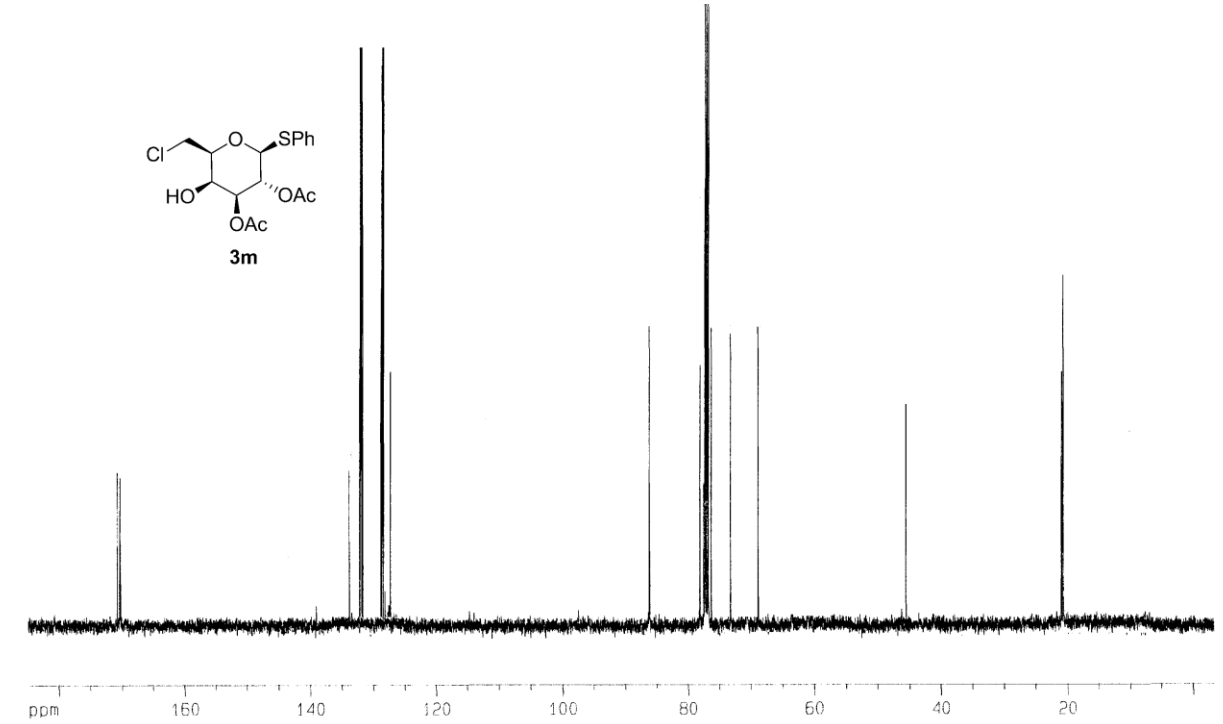


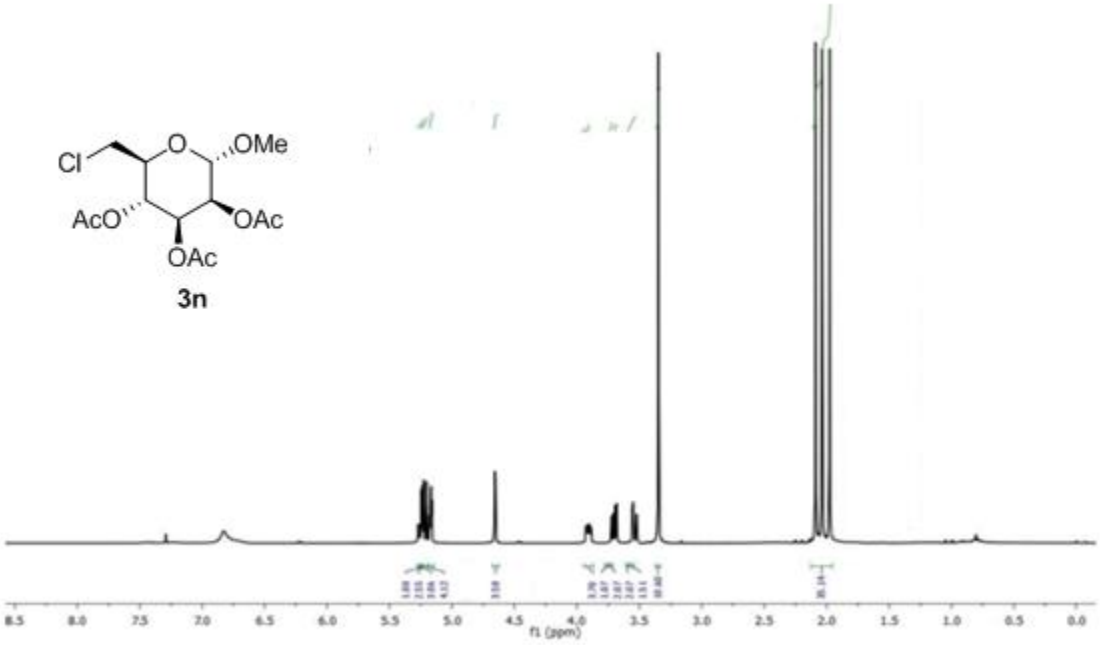


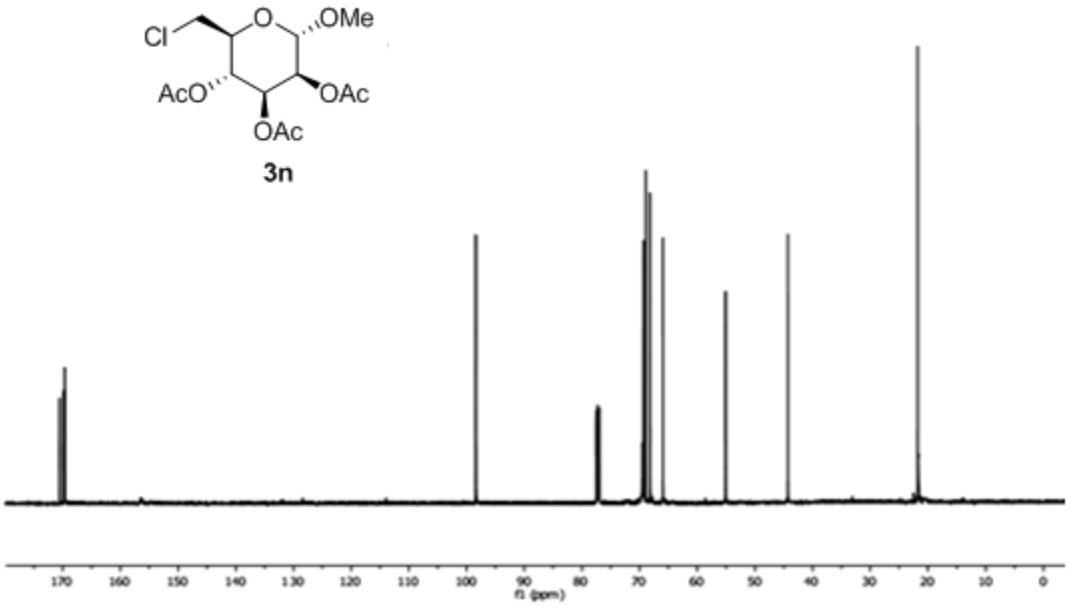


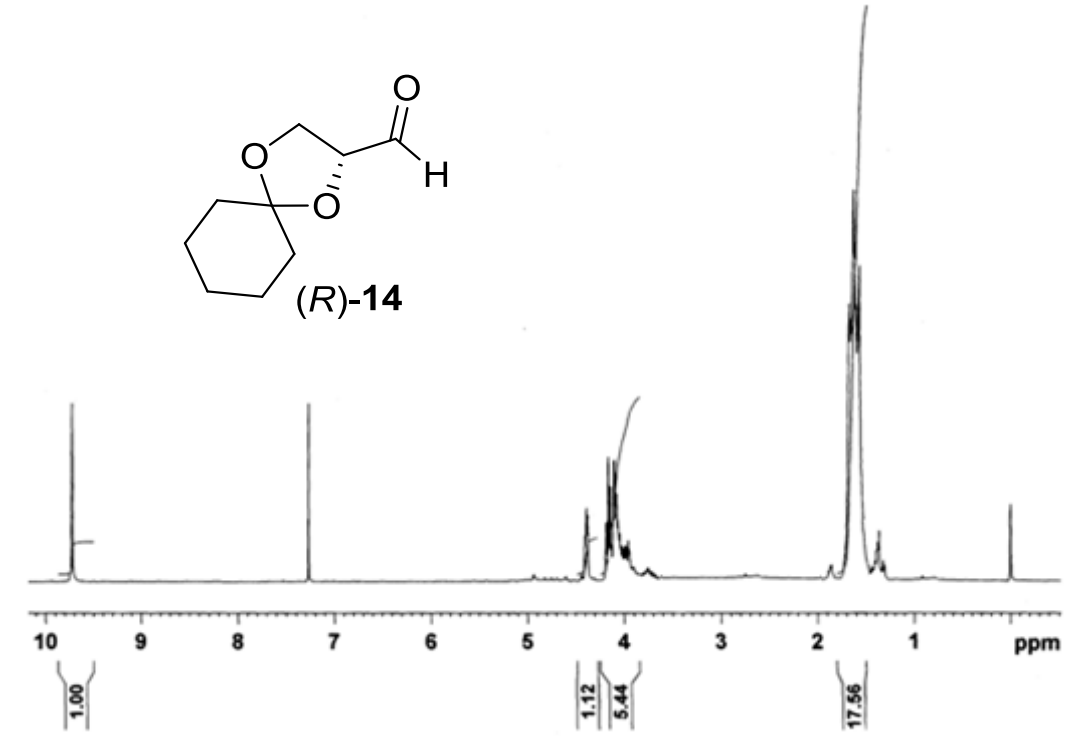


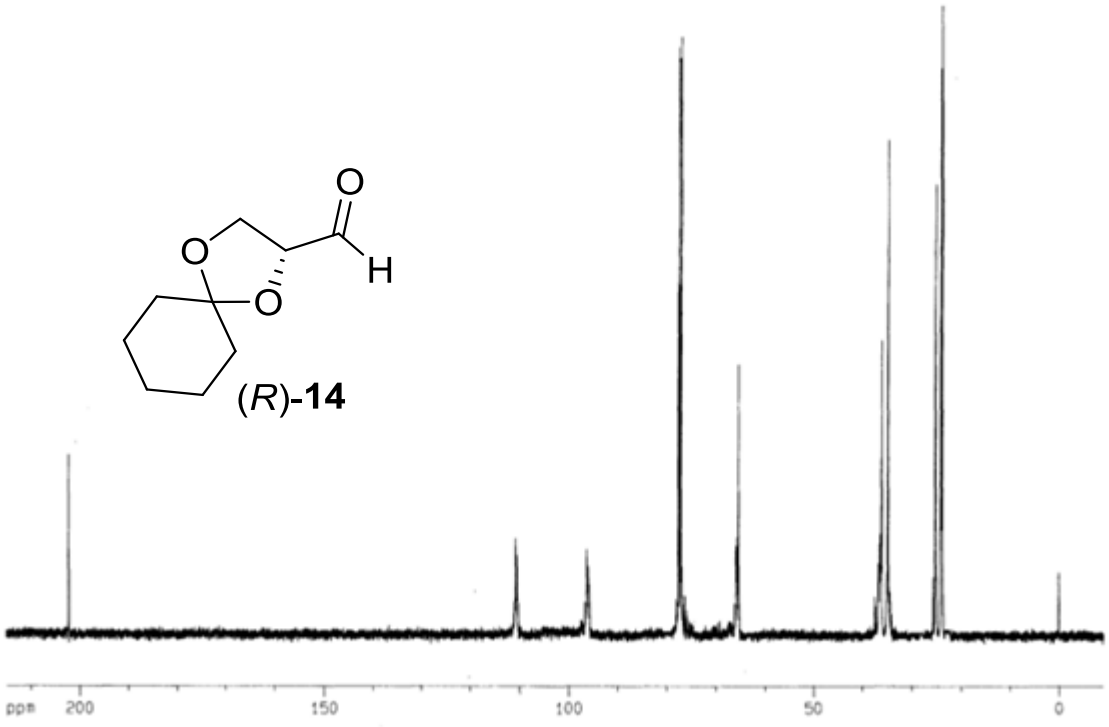


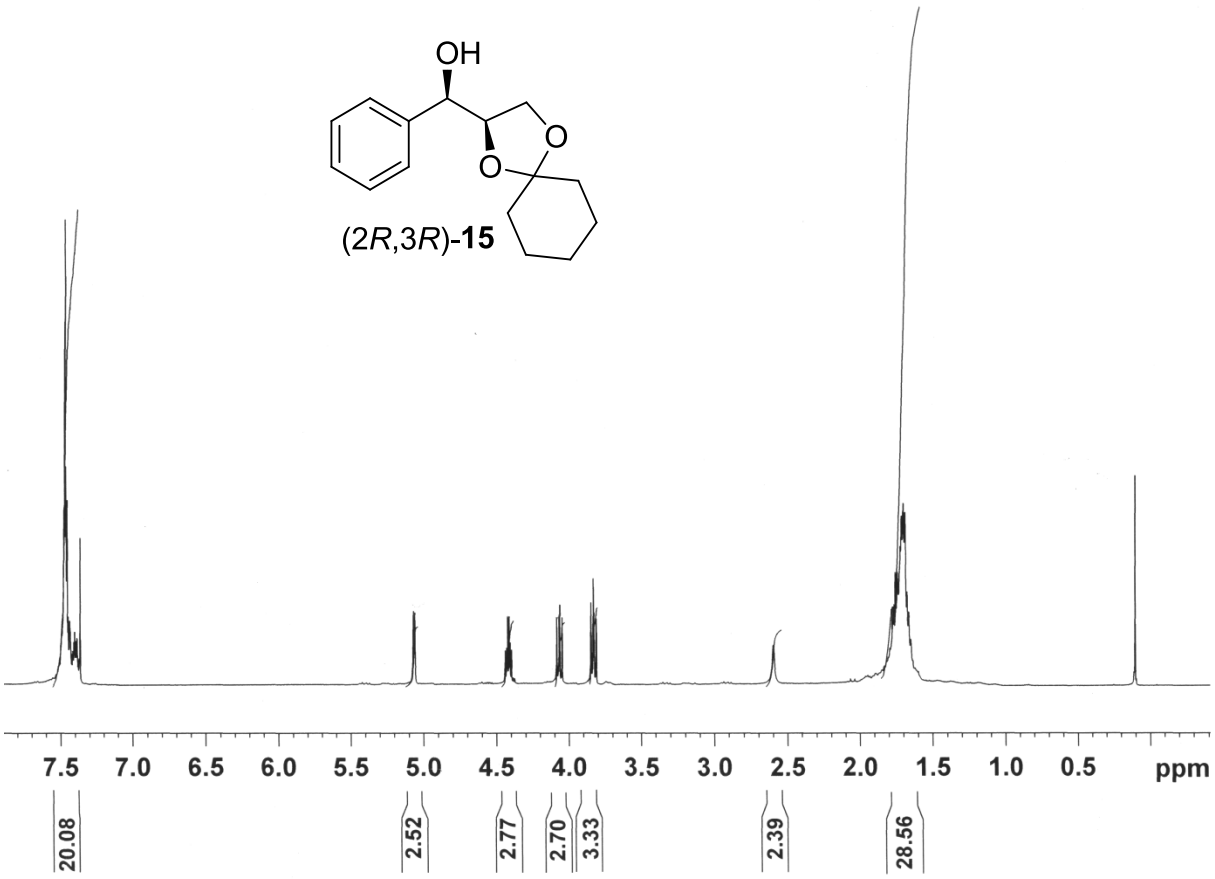


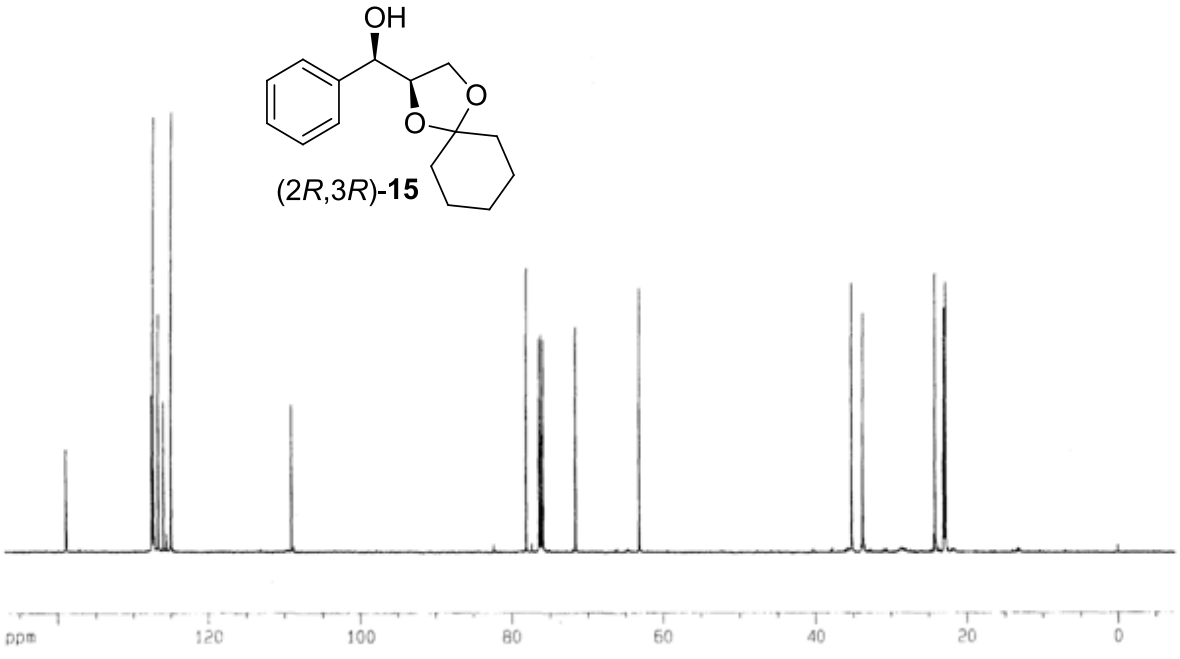


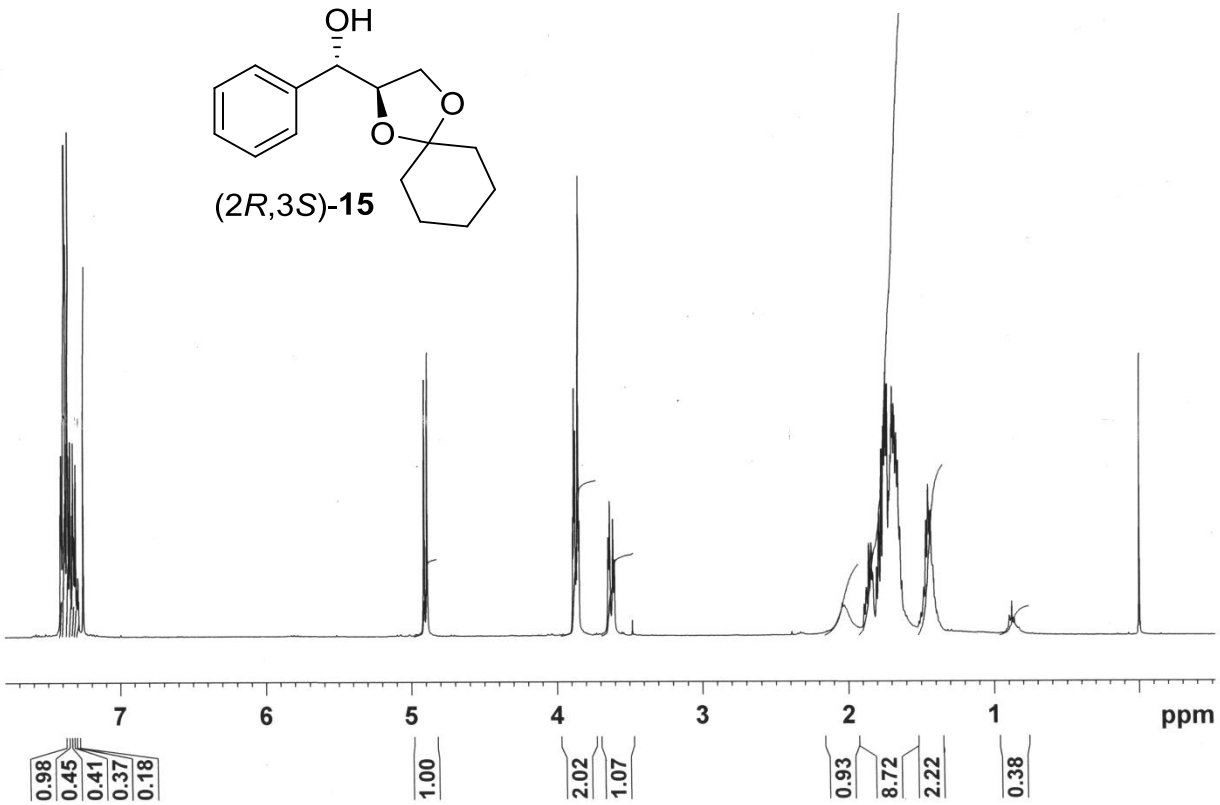


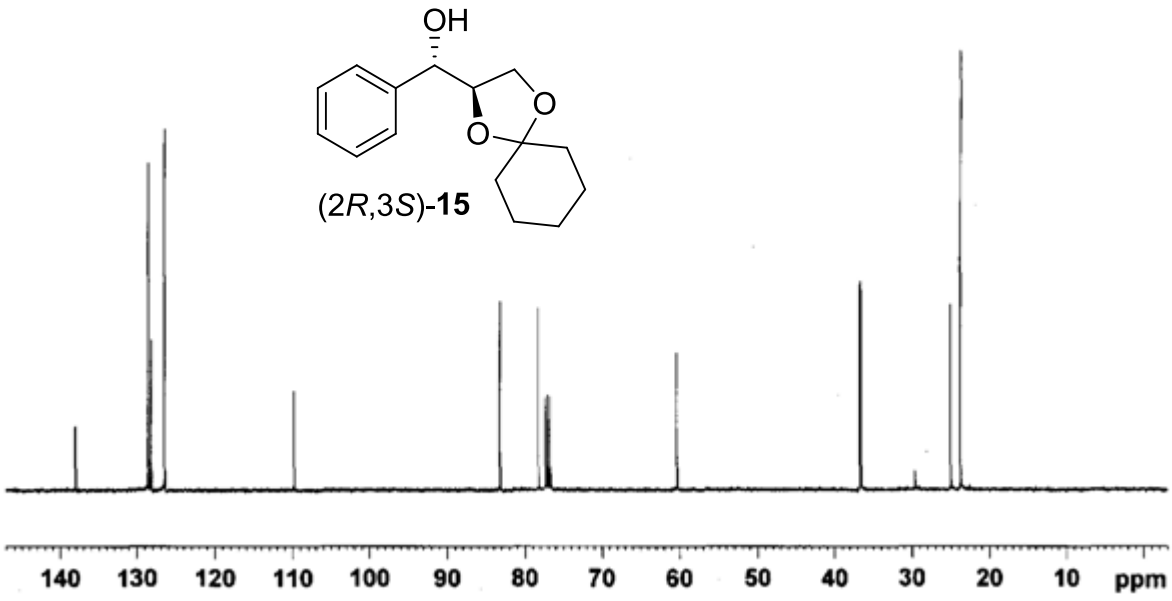


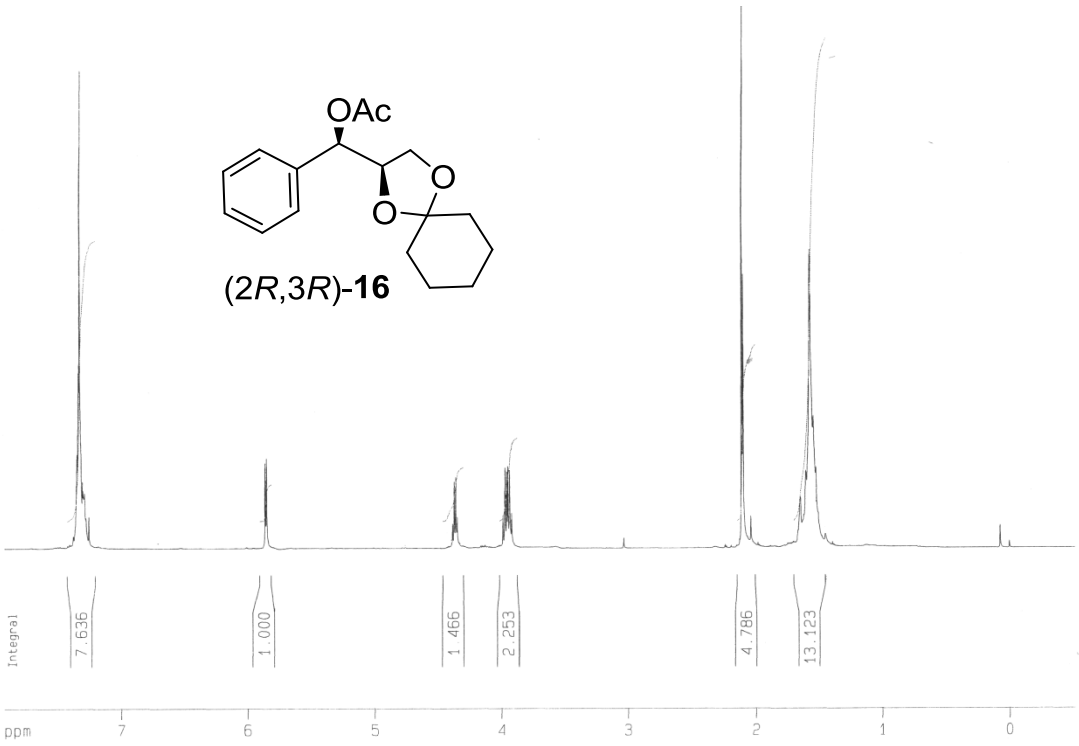


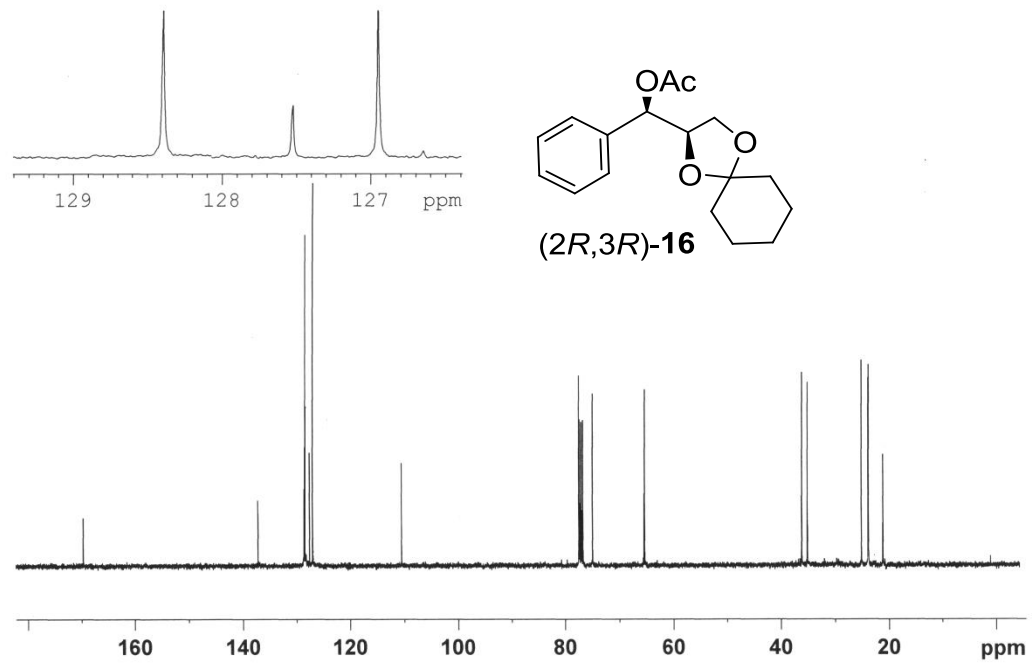


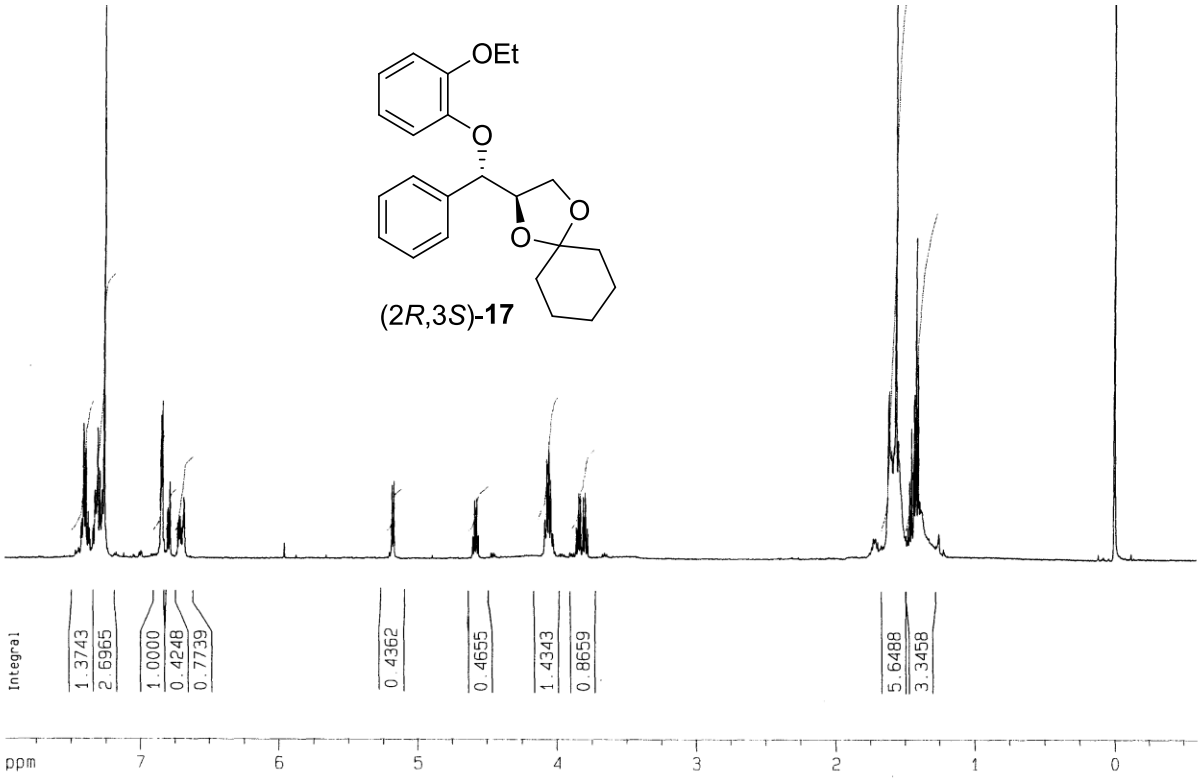


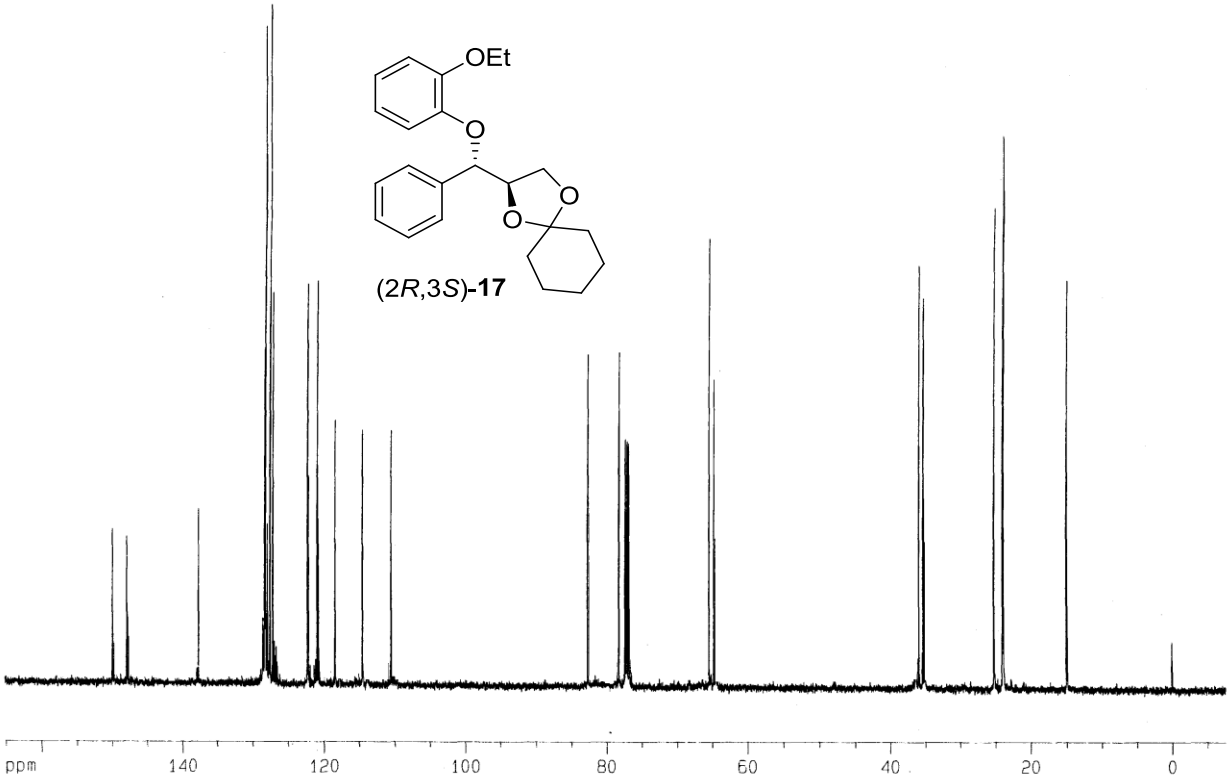


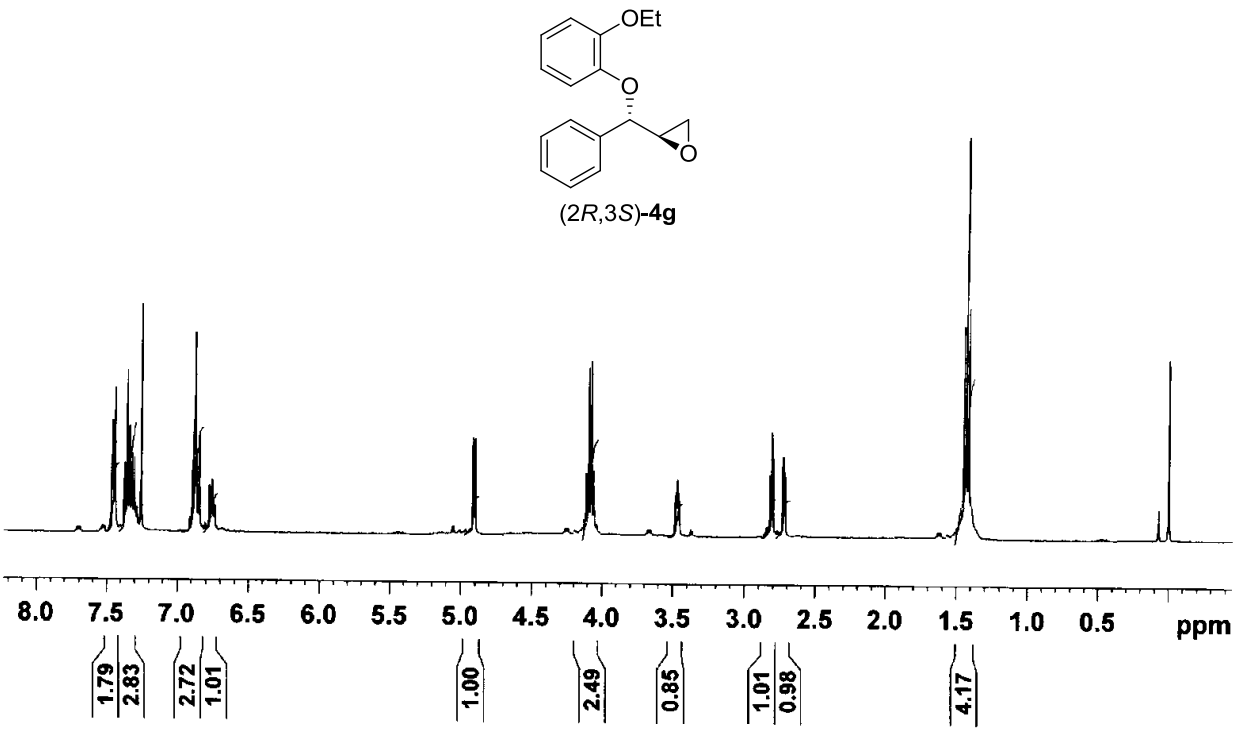


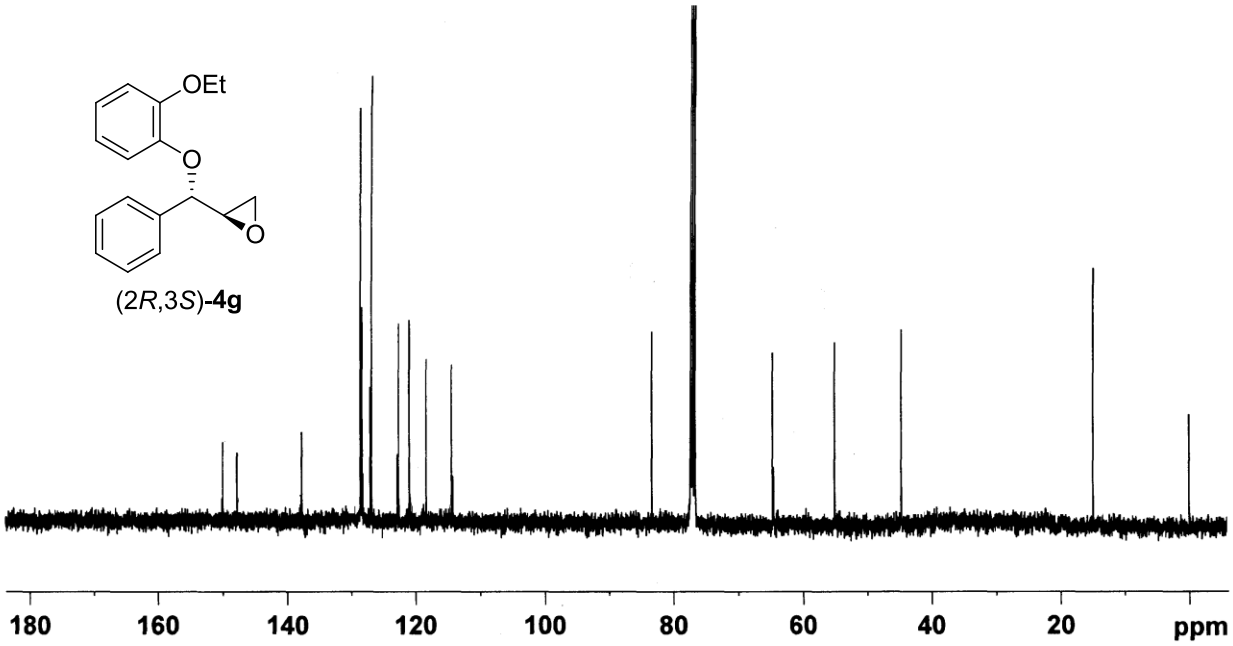


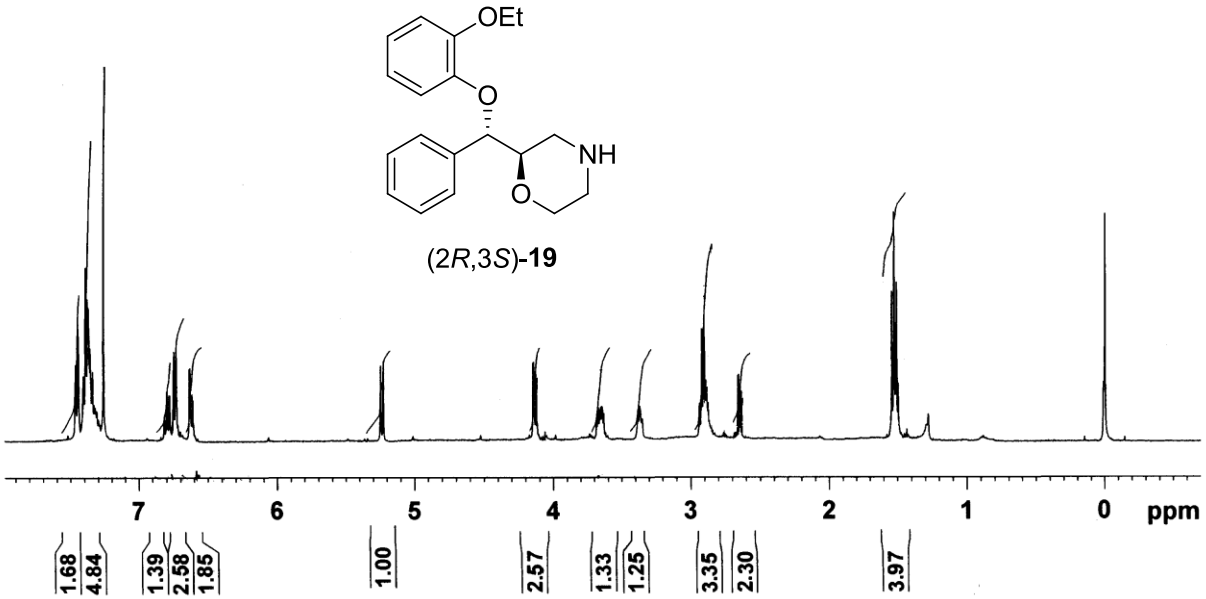




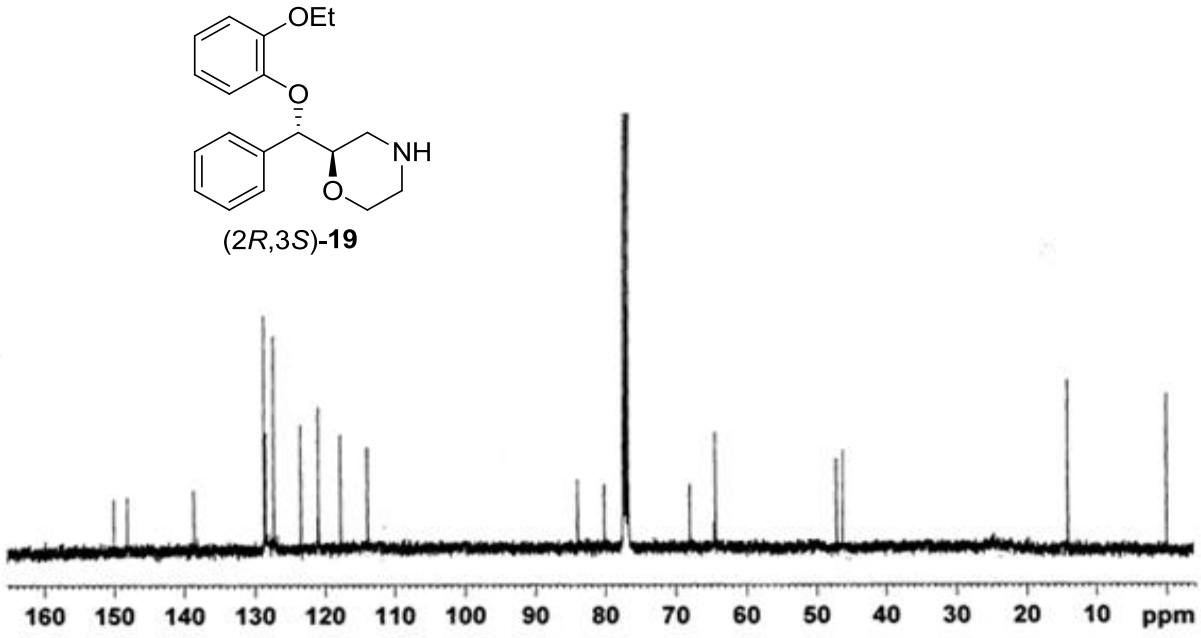








(2*R*,3*S*)-**19**



(2*R*,3*S*)-**19**