Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information

Nonhydrolyzable Analogs of Phosphatidylinositol as Ligands of Phospholipases C

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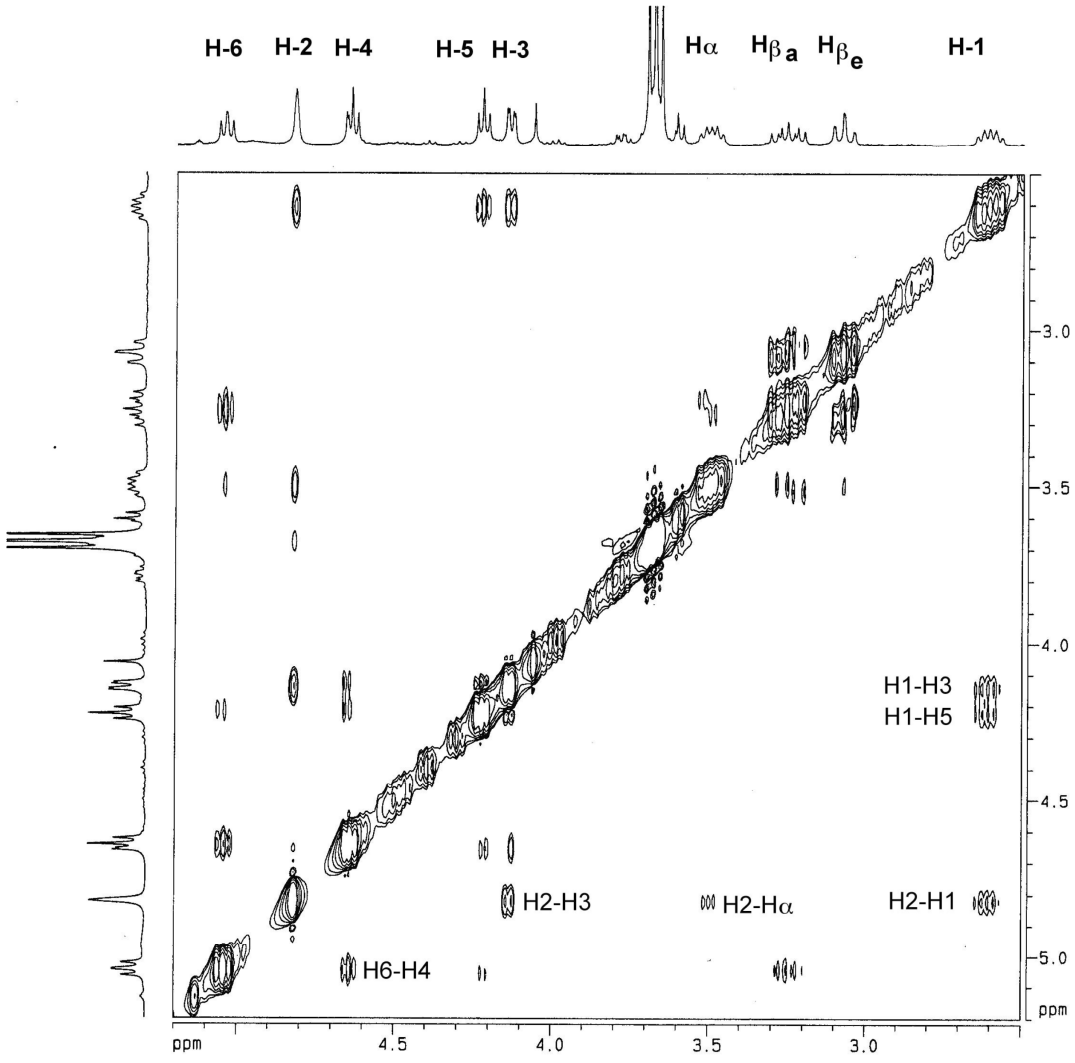

Figure 1. 500 MHz NOESY spectrum of the lactone **23** in Py-d_5; mixing time 250 ms.

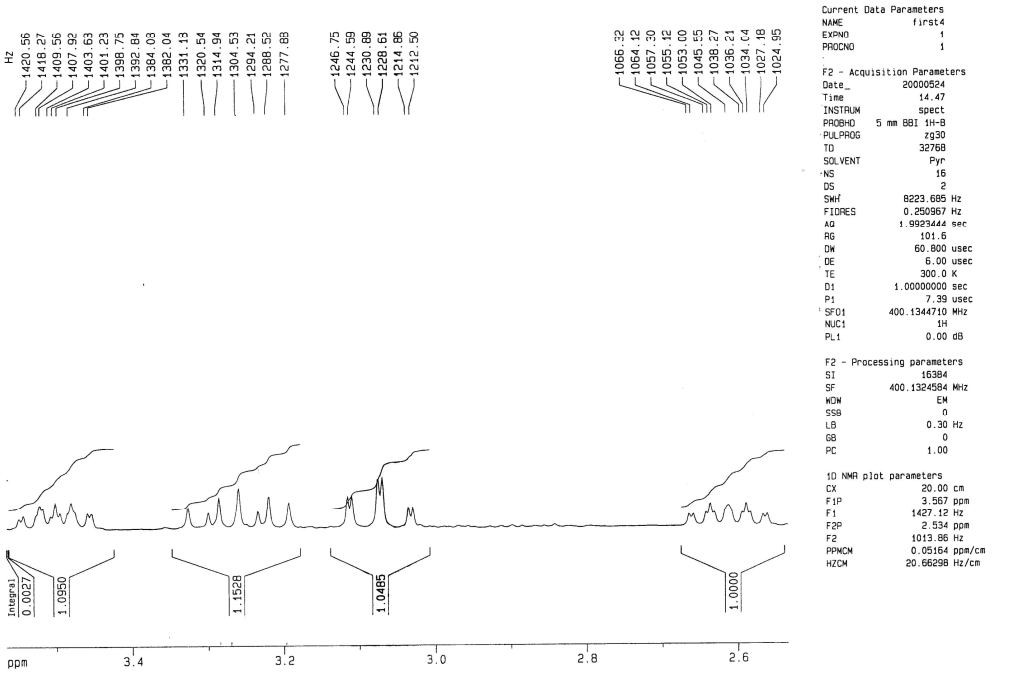

Figure 2. Expanded partial 400 MHz ^{1}H NMR spectrum of lactone **23** in pyridine-d_6.

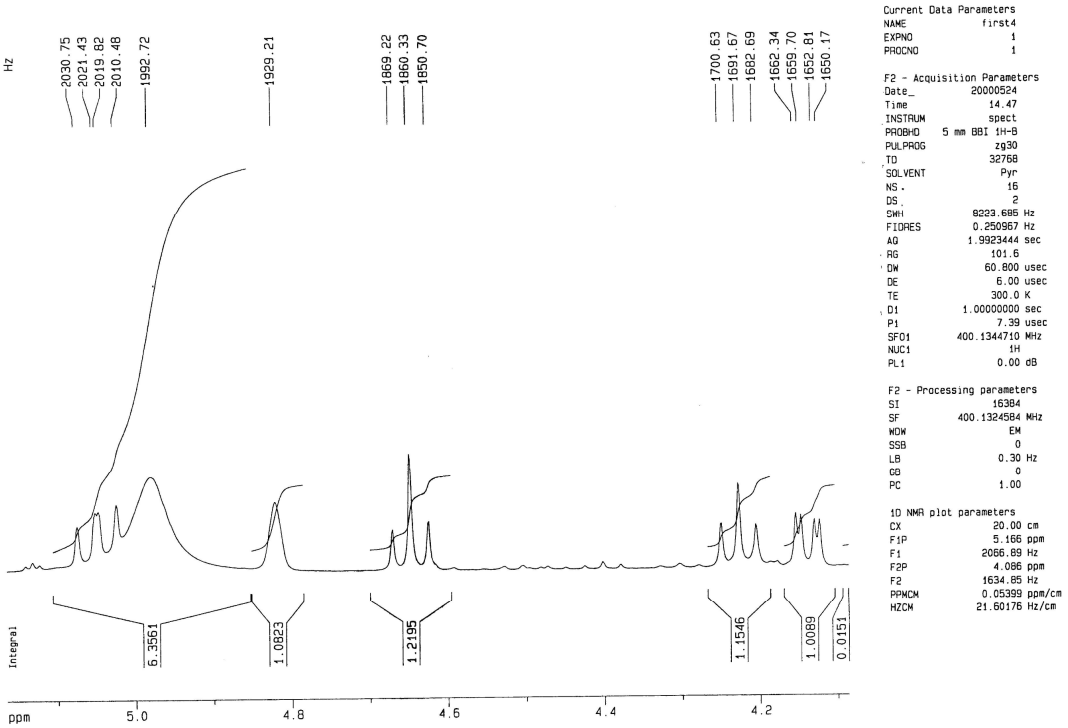

Figure 3. Expanded partial 400 MHz ^{1}H NMR spectrum of lactone **23** in pyridine-d_6.

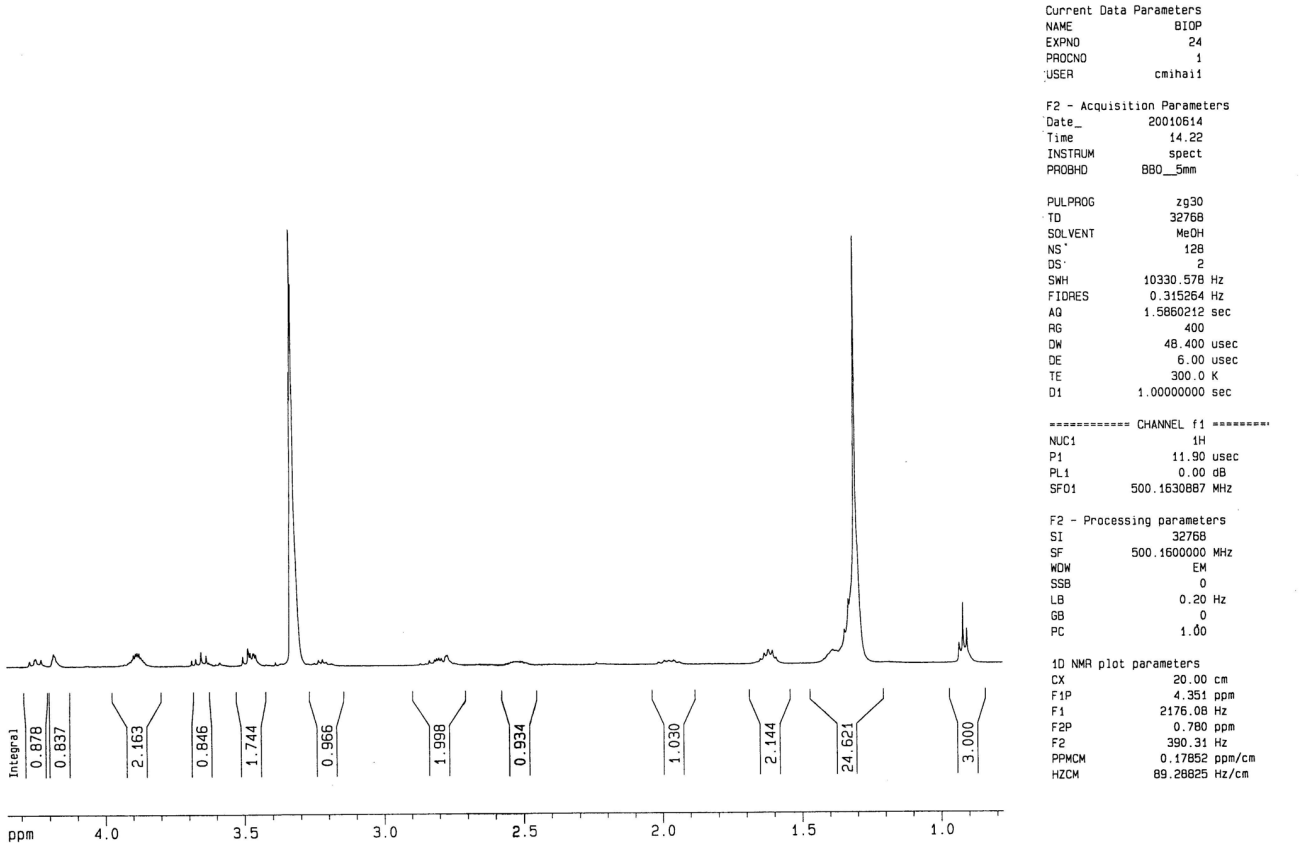

Figure 4. 500 MHz ^{1}H NMR spectrum of ligand **10** in methanol-d_4.

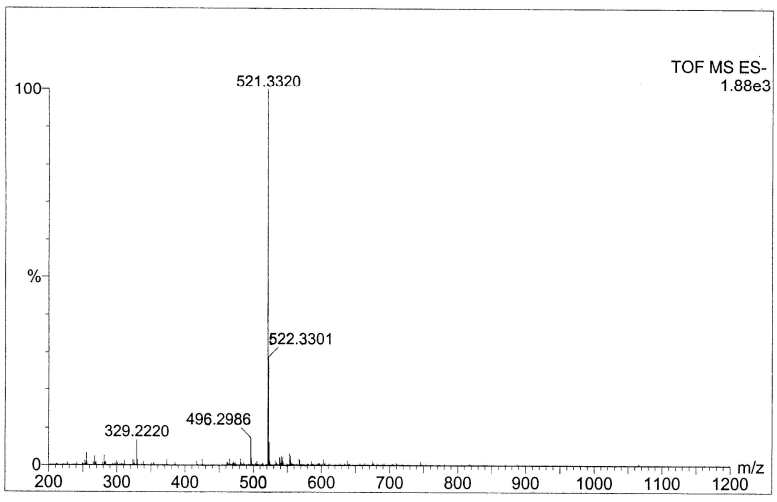

Figure 5. HR ES MS spectrum of ligand **10**.

(2*R*)-3-*O*-Benzyl-1,2-di-*O*-hexyl-*sn*-glycerol (**25**). A suspension of (*R*)-3-benzyloxy-1,2-propanediol (1g, 5.5 mmol), 1-bromohexane (3.6 g, 22 mmol) and powdered potassium hydroxide (1.23 g, 22 mmol) in toluene (25 mL) was heated at reflux using a Dean-Stark drying tube for 24 hours. When reaction was complete (TLC in hexane-ethyl acetate, 4:1), the reaction mixture was cooled at room temperature and washed twice with water. The organic extract was concentrated and the residue was purified by chromatography (hexane-ethyl acetate, 8:1) to afford pure **25** (1.8 g, 95%) as colorless oil. R_f = 0.75 (hexane-ethyl acetate, 4:1); ^{1}H NMR ($CDCl_3$) δ 0.85 (t, 6H), 1.28-1.49 (m, 12H), 1.52-1.61 (m, 4H), 3.44 (t, 2H), 3.48-3.64 (m, 7H), 4.54 (s, 2H), 7.21-7.32 (m, 5H); ^{13}C NMR ($CDCl_3$) δ 14.13, 22.73, 25.87, 25.89, 29.72, 30.16, 31.78, 31.80, 70.36, 70.66, 70.82, 71.69, 73.41, 78.02, 127.54, 127.62, 128.35, 138.53.

(2*R*)-1,2-Di-*O*-hexyl-*sn*-glycerol (**17**). Into the solution of **17** (1.67 g, 4.8 mmol) in dry methanol (25 mL) was added palladium on charcoal (300 mg). The mixture was shaken in Parr apparatus overnight. The subsequent fltration of catalyst through a layer of Celite and concentration afforded pure **17** (1.2 g, 97%) as colorless oil. R_f = 0.35 (hexane-ethyl acetate, 3:1); ^{1}H NMR ($CDCl_3$) δ 0.82 (t, 6H), 1.14-1.25 (m, 12H), 1.51 (m, 4H), 2.48 (br s, 1H), 3.37-3.65 (m, 9H).