Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Synthesis and properties of a series of β-cyclodextrin / nitrone spin traps for improved superoxide detection

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TABLE OF CONTENTS

EXPERIMENTAL PROCEDURES

Materials

CH_2Cl_2 was distilled under dry argon atmosphere in the presence of P_2O_5. All reagents were used as received without further purification. The reactions were monitored by TLC on silica gel Merck $60F_{254}$ and by ^{31}P NMR. Crude materials were purified by flash chromatography on Merck Silica gel 60 (0.040-0.063 mm). ^{31}P NMR, ^{1}H NMR and ^{13}C NMR spectra were recorded with a Bruker DPX 300 or 400 spectrometers at 121.49, 300.13 and 75.54 MHz respectively. ^{31}P NMR was taken in $CDCl_3$ using 85% H_3PO_4 as an external standard with broad-band ^{1}H decoupling. ^{1}H NMR and ^{13}C NMR were taken in $CDCl_3$ using TMS or $CDCl_3$ as internal reference respectively. Chemical shifts (δ) are reported in ppm and coupling constant *J* values in Hertz. The assignments of NMR signals were facilitated by use of the DEPT 135 sequence. Mass Spectrometry analyses were determined at the Spectropole faculty of the Aix-Marseille Université (amu). DIPPMPO was obtained from Radical Vision (Marseille, France). HPLC/MS experiments were performed using an Agilent 1260 infinity system coupled with a 6120 simple quadripole. This system is equipped with a C18 column (Zorbax 1.8 μM, 3 × 50 mm) that was equilibrated with 10% CH_3CN (containing 0.1% (v/v) formic acid) in 0.1% formic acid aqueous solution at the flow rate of 0.5 mL/min. After sample injection the CH_3CN mobile phase concentration raised to 40% after 3 min. Then, raised to 100% after 8 min. This concentration is maintained over a period of 6 min.

The synthesis was performed adapting the procedure described by Hardy et al.[1]

Synthesis of the nitrone NHS-BEPMPO X

The preparation of nitrophosphonate **4** was performed adapting the procedure described by Friedrich et al.[2] and Hardy et al.[1]

*Butyl-ethyl-(1-nitroethyl)-phosphonate **4**.*

^{31}P NMR (121.49 MHz) δ 13.40 (50%), 13.33 (50%); ^{1}H NMR (300.13 MHz) δ 0.93 (3H, t, *J* = 7.3), 1.31-1.44 (5H, m), 1.71-1.63 (2H, m), 1.80 (3H, dd, *J* = 7.3, 16.3), 4.27-4.12 (4H, m), 4.94-5.03 (1H, m). ^{13}C NMR (75.47 MHz) δ 79.28 (d, *J* = 143.8), 79.25 (d, *J* = 144.5), 67.8 (d, *J* = 7.3), 67.6 (d, *J* = 6.6), 64.3 (d, *J* = 6.6), 64.1 (d, *J* = 6.6), 32.3 (d, *J* = 5.9), 32.2 (d, *J* = 5.9), 18.4 (d, *J* = 2.9), 16.2 (d, *J* = 5.9), 16.1 (d, *J* = 5.9), 14.3 (d, *J* = 3.7), 13.4 (s). LC-MS: m/z: 240.2 $[M + H]^+$, retention time: 6.32 min.

*4-(1-Ethoxy-1-butoxyphosphoryl-1-nitroethyl)-tetrahydrofuran-2-one **5**.*

The product **5** was obtained as a yellow oil (80%) corresponding to a mixture of four diastereoisomers. ^{31}P NMR (121.49 MHz) δ 14.56 (25%), 14.54 (25%), 14.48 (25%), 14.45 (25%). ^{1}H NMR (300.13 MHz) δ 0.93, 0.94 (3H, 2t, *J* = 7.3, 7.5), 1.32-1.44 (5H, m), 1.63-1.72 (2H, m), 1.79, 1.80 (3H, 2d, *J* = 14.6, 14.3), 2.43-2.81 (2H, m), 3.68-3.78 (1H, m), 4.10-4.30 (4H, m), 4.35-4.54 (2H, m). ^{13}C NMR (75.47 MHz) δ 174.64, 174.62, 174.49, 174.47 (1C, 4s), 90.5, 90.4, 90.2, 90.1 (1C, 4d, *J* = 147.5, 147.5, 146.7, 146.7), 68.1-68.7 (1C, m), 65.2, 65.1, 65.0 (1C, 3d, *J* = 7.3, 7.3, 7.3), 40.3 (1C, s), 39.8 (1C, s), 32.3 (1C, 2d, *J* = 5.9), 30.2, 29.9 (1C, d, s, *J* = 8.1), 18.6 (1C, s), 16.2-16.4 (2C, m), 13.4 (1C, s). LC-MS: m/z: 324.2 $[M + H]^+$, retention time: 6.36 min.

*4-(1-Ethoxy-1-butoxyphosphoryl-1-nitroethyl)-2-hydroxytetrahydrofurane **6**.*

The product **6** was obtained as a yellow oil (55%) corresponding to a mixture of eight diastereoisomers.

^{31}P NMR (121.49 MHz) δ 15.88, 15.90, 16.04, 16.2, 16.3; ^{1}H NMR (300.13 MHz) δ 0.93 (3H, t, *J* = 7.3), 1.32-1.42 (5H, m), 1.63-1.69 (2H, m), 1.75, 1.83 (3H, 2d, *J* = 14.3, 14.6),

1.91-2.19 (2H, m), 3.63-3.71 (1H, m), 3.82-4.00 (2H, m), 4.05-4.28 (4H, m), 5.51-5.57 (1H, m). ^{13}C NMR (75.47 MHz) δ 98.74, 98.71, 98.54, 98.50 (1C, 4s), 91.5 (1C, d, *J* = 149.7), 68.0 (1C, 2d, *J* = 7.3, 7.3), 67.2 (1C, d, *J* = 8.8), 64.4-64.75 (1C, m), 42.4, 42.1 (1C, 2s), 35.7, 35.6 (1C, s, d, *J* = 2.2), 32.4 (1C, s), 18.6 (1C, s), 16.4, 15.9 (2C, d, s, *J* = 4.4), 13.5 (1C, s). LC-MS: m/z: 650.6 $[M]^{2+}$, retention time: 5.72 min.

(4R, 5R*)-5-Ethoxy-(R,S)-butoxyphosphoryl-5-methyl-4-hydroxymethyl-1-pyrroline N-Oxide **7**.*

The nitrones **7** were obtained in 55% yield corresponding to a mixture of 4 diastereoisomers. The cis isomers were purified.

(4R*, 5R*)-4-HMBEPMPO **7**; ^{31}P NMR (121.49 MHz) δ 22.5, 22.6; ^{1}H NMR (300.13 MHz) δ 0.86 (3H, 2t, *J* = 7.3, 7.5), 1.25-1.39 (5H, m), 1.56-1.64 (2H, m), 1.67, 1.68 (3H, 2d, *J* = 14.8, 14.6), 2.38-2.67 (3H, m), 3.82 (2H, d, *J* = 5.8), 4.0-4.28 (4H, m), 6.87 (1H, s); ^{13}C NMR (75.47 MHz) δ 133.7 (1C, 2d, *J* = 8.8, 8.8), 76.1, 76.0 (1C, 2d, *J* = 150.4, 149.7), 66.5, 66.3 (1C, 2d, *J* = 7.3, 7.3), 63.1, 62.9 (1C, 2d, *J* = 6.6, 7.3), 61.3 (1C, d, *J* = 5.1), 48.3 (1C, 2d, *J* = 3.7, 2.9), 31.5 (1C, 2d, *J* = 5.9, 5.6), 28.4 (1C, d, *J* = 8.8), 20.4, 20.3 (1C, 2d, *J* = 1.5, 1.5), 17.7 (1C, d, *J* = 8.1), 15.4, 15.4 (1C, 2d, *J* = 5.1, 5.9), 12.6 (1C, s); LC-MS: m/z: 294.2 $[M + H]^{+}$, retention time: 3.98 min.

(4R, 5R*)-5-Ethoxy-(R,S)-butoxyphosphoryl-5-methyl-4-(succinimidyloxycarbonyl-oxymethyl)-1-pyrroline N-Oxide **8**.*

The nitrones **8** were obtained in 95% yield corresponding to a mixture of 4 diastereoisomers. The cis isomers were purified.

(4R*, 5R*)-NHS-BEPMPO **8**; ^{31}P NMR (121.49 MHz) δ 18.7, 18.8; ^{1}H NMR (300.13 MHz) δ 0.83 (3H, t, *J* = 6.6), 1.21-1.34 (5H, m), 1.52-1.64 (2H, m), 1.61 (3H, d, *J* = 13.8), 2.54-2.82

(3H, m), 2.75 (4H, s), 3.99-4.18 (4H, m), 4.44-4.52 (1H, m), 4.61-4.70 (1H, m), 6.89 (1H, dt, *J* = 3.0, 2.9); ^{13}C NMR (75.47 MHz) δ 168.5 (1C, s), 151.0 (1C, s), 133.8 (1C, 2d, *J* = 7.7, 7.7), 75.9, 75.8 (1C, 2d, *J* = 148.7, 148.7), 69.9 (1C, d, *J* = 2.7), 68.0, 64.5 (1C, 2d, *J* = 6.6, 6.6), 66.3, 62.8 (1C, 2d, *J* = 7.7, 7.7), 45.4 (1C, 2d, *J* = 2.2, 2.2), 32.3, 32.0 (1C, 2d, *J* = 6.0, 6.0), 29.7 (1C, d, *J* = 5.5), 25.2 (2C, s), 20.0 (1C, s), 18.4 (1C, s), 16.2 (1C, d, *J* = 6.0), 16.0 (1C, d, *J* = 5.5), 13.3 (1C, d, *J* = 6.6). LC-MS: m/z: 435.2 $[M + H]^+$, retention time: 5.04 min.

*Synthesis of the nitrone CD-BEPMPO **9**.*

To a mixture of NHS-BEPMPO (0.107 g, 0.25 mmol) and permethyl CD-NH_2 (0.358 g, 0.25 mmol) in CH_2Cl_2 (5 mL) was added triethylamine (77 μL, 0.55 mmol) at room temperature under argon. The reaction mixture was stirred for 3 h. Then, $CHCl_3$ (100 mL) is added to the mixture and washed with water (2×10 mL). The organic layer was dried over Na_2SO_4 and the solvent distilled under reduced pressure. Purification of the crude product by flash chromatography on a silicagel (CH_2Cl_2/EtOH 90:10) afforded a white powder, corresponding to CD-BEPMPO **9** (0.28 g, 64%).

^{31}P NMR (121.49 MHz, $CDCl_3$) δ 19.43, 19.39. ^{1}H NMR (300.13 MHz, $CDCl_3$) δ 6.98-6.98 (m, 1H), 5.39-5.31 (m, 1H), 5.15-5.02 (m, 7H), 4.60-4.49 (m, 1H), 4.32-4.03 (m, 5H), 3.86-3.28 (m, 95H), 3.21-3.11 (m, 7H), 2.78-2.53 (m, 3H), 1.68 (d, 3H, *J* = 13.9), 1.45-1.25 (m, 7H), 0.96-0.88 (m, 3H).

^{13}C NMR (75.47 MHz) δ 156.3 (C, s), 134.6 (C, d, *J* = 6), 99.2-98.4 (7C, m), 82.1-79.7 (21C, m), 76.0 (1C, d, *J* = 198), 71.7-70.8 (13C, s), 66.2 (1C, d, *J* = 6.6), 64.5 (1C, d, *J* = 6.6), 61.6-61.1 (6C, m), 59.3-58.3 (14C, m), 46.7 (1C, s), 41.6 (C, d, *J* = 6), 32.3 (1C, d, *J* = 6), 30.6 (C, s), 22.3 (1C, s), 20.3 (C, s), 18.7 (1C, s), 16.4 (C, d, *J* = 6), 13.6 (C, d, *J* = 7.3). HMRS calcd. for $[C_{75}H_{133}N_3O_{40}P]$; $[C_{75}H_{133}N_3O_{40}P]^{++}$ 875.9292, found: 875.9287.

*Synthesis of the nitrone CD_6-DEPMPO **10**.*

Compound **A**. To a mixture of tert-butyl-(3-hydroxy-propyl)-carbamate (0.5 g, 2.8 mmol) and DSC (0.88 g, 3.4 mmol) in 5 mL of acetonitrile was added at 0°C TEA (0.412 mL, 2.8 mmol) under argon. After 3 hours of reaction, the solvent is distilled under reduced pressure. Purification of the crude product was performed by flash chromatography on a silicagel (Et_2O/CH_2Cl_2, 70:30) afforded the compound **A** (0.7 g, 80%).

Compound **B**. To a mixture of compound **A** (0.1 g, 0.3 mmol) with the permethyl βCD-NH_2 (0.477 g, 0.3 mmol) in CH_2Cl_2 (7 mL) was added TEA (0.100 mL, 0.7 mmol) at 0°C. The reaction mixture was stirred for 6 h. The mixture was diluted with 100 mL of CH_2Cl_2 and washed with water (20 mL), $NaHCO_3$ (20 mL) and brine (20 mL). The organic layer was dried over Na_2SO_4 and the solvent distilled under reduced pressure. Purification of the crude product by flash chromatography on a silicagel (CH_2Cl_2/EtOH 90:10) afforded a white powder, corresponding to compound **B** (0.5 g, 93%).

Compound **C**. To a mixture of compound **B** (0.5 g) in CH_2Cl_2 was added at 0°C TFA (1 mL). The reaction mixture was stirred 1h and afforded a white powder, corresponding to compound **C** (CD_6-NH_2, 0.4 g).

CD_6-DEPMPO. To a mixture of NHS-DEPMPO (0.08 g, 1.97 mmol) and permethyl CD_6-NH_2 (0.286 g, 1.97 mmol) in CH_2Cl_2 (10 mL) was added triethylamine (55 mL, 3.94 mmol) at room temperature under argon. The reaction mixture was stirred for 3 h and then washed with water (2 × 15 mL). The organic layer was dried over Na_2SO_4 and the solvent distilled under reduced pressure. Purification of the crude product by flash chromatography on a silicagel (CH_2Cl_2/EtOH 90:10) afforded a white powder, corresponding to CD_6-DEPMPO (0.27 g, 80%).

^{31}P NMR (121.49 MHz, $CDCl_3$) δ 19.72. ^{1}H NMR (300.13 MHz, $CDCl_3$) δ 6.99 (td, 1H, J = 6.1), 5.47-5.32 (m, 1H), 5.20-5.02 (m, 7H), 4.59-4.48 (m, 1H), 4.35-4.08 (m, 7H), 3.92-3.06

(m, 104H), 2.82-2.54 (m, 3H), 1.81 (1H, m), 1.87-1.75 (2H, m), 1.70 (d, 3H, , J = 14.0), 1.32 (dt, 6H, , J = 7.2, 6.9). ^{13}C NMR (75.47 MHz) δ 156.9 ($1C^{IV}$, s), 155.9 ($1C^{IV}$, s), 134.5 (1C, d, *J* = 7.5), 99.0-98.3 (7C, m), 82.1-79.6 (21C, m), 76.0 ($1C^{IV}$, d, *J* = 174.4), 71.6-70.6 (13C, s), 64.2 (1C, d, *J* = 6.3), 63.9 (1C, s), 62.3 (1C, d, *J* = 7.5), 61.6 (1C, s), 61.5-60.9 (6C, m), 59.2-58.0 (14C, m), 46.5 (1C, s), 37.3 (1C, s), 33.9 (1C, s), 33.5 (1C, s), 30.2 (1C, s), 20.1 (1C, s), 16.2 (1C, d, *J* = 5.7), 16.1 (1C, d, *J* = 6.3).

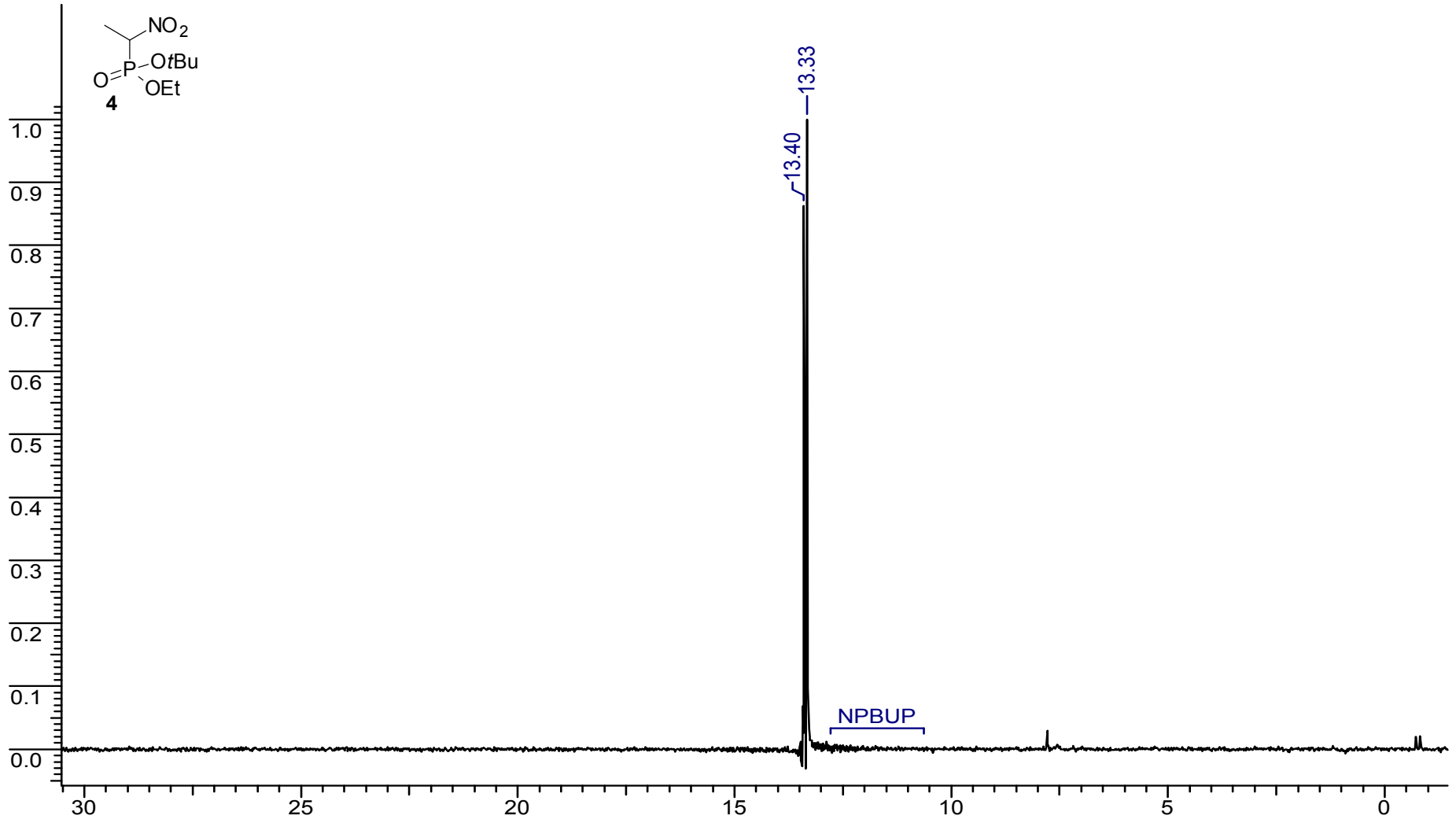
*Synthesis of the nitrone CD-DIPPMPO **11**.*

To a mixture of NHS-DIPPMPO (0.2 g, 0.46 mmol) and permethyl CD-NH_2 (0.71 g, 0.46 mmol) in CH_2Cl_2 (15 mL) was added at room temperature under inert atmosphere triethylamine (141 μL, 1.06 mmol). The reaction mixture was stirred for 3 h. The solution was washed twice with 10 ml of distilled water and extracted three times with 100 mL of $CHCl_3$. The organic layers were collected and dried over Na_2SO_4 and the solvent distilled under reduce pressure. Purification of the crude product by flash chromatography on silicagel (CH_2Cl_2/EtOH 80:20) afforded a white powder (0.46 g, 58 %), corresponding to CD-DIPPMPO **11**.

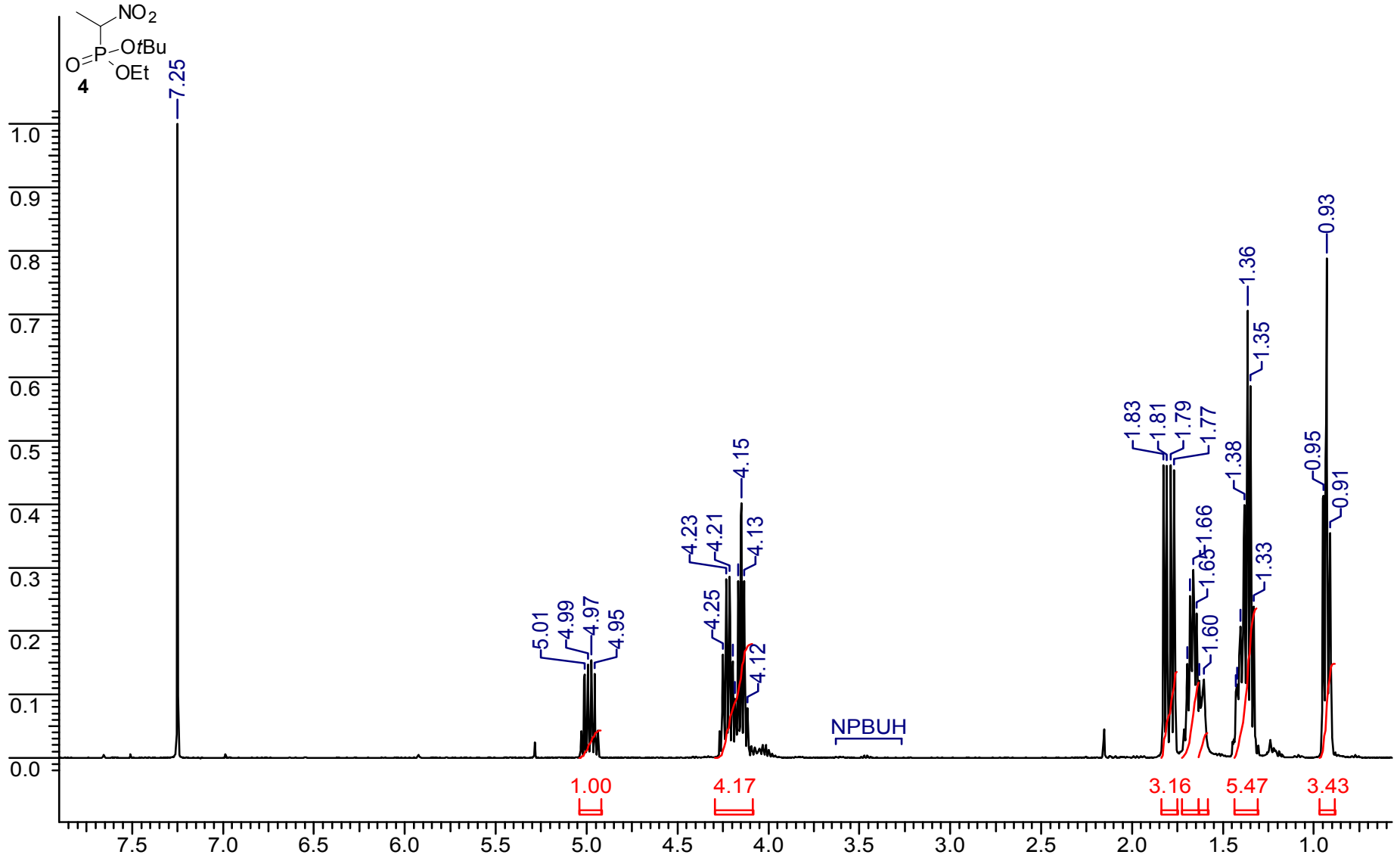
^{31}P NMR (121.49 MHz, $CDCl_3$) δ 17.65. ^{1}H NMR (300.13 MHz, $CDCl_3$) δ 6.97-6.91 (m, 1H), 5.37-5.30 (m, 1H), 5.15-5.02 (m, 7H), 4.80-4.67 (m, 2H), 4.56-4.45 (m, 1H), 4.30-4.17 (m, 1H), 3.86-3.28 (m, 95H), 3.19-3.11 (m, 7H), 2.75-2.53 (m, 3H), 1.60 (d, 3H, *J* = 13.8), 1.40-1.25 (m, 12H). ^{13}C NMR (75.47 MHz) δ 156.3 (C^{IV}, s) 134.1 (C, d, *J* = 8), 99.0-98.4 (C, m), 82.1-79.6 (C, m), 76.0 (C^{IV}, d, *J* = 150.1),73.1 (C, s), 71.6-70.6 (C, s), 64.5 (C, s), 61.5-60.9 (C, m), 59.2-58.0 (C, m), 46.5 (C, s), 41.4 (C, d, *J* = 8), 30.6 (C, s), 24.5 (C, s), 23.6 (C, d, *J* = 3.4), 23.7 (C, d, *J* = 5.1), 23.4 (C, d, *J* = 6.0), 20.3 (C, s). HMRS calcd. for $[C_{75}H_{133}N_2O_{40}P]$; $[C_{75}H_{133}N_2O_{40}P]^{++}$, 875.9292 found: 875.9288.

NMR SPECTRA OF COMPOUNDS

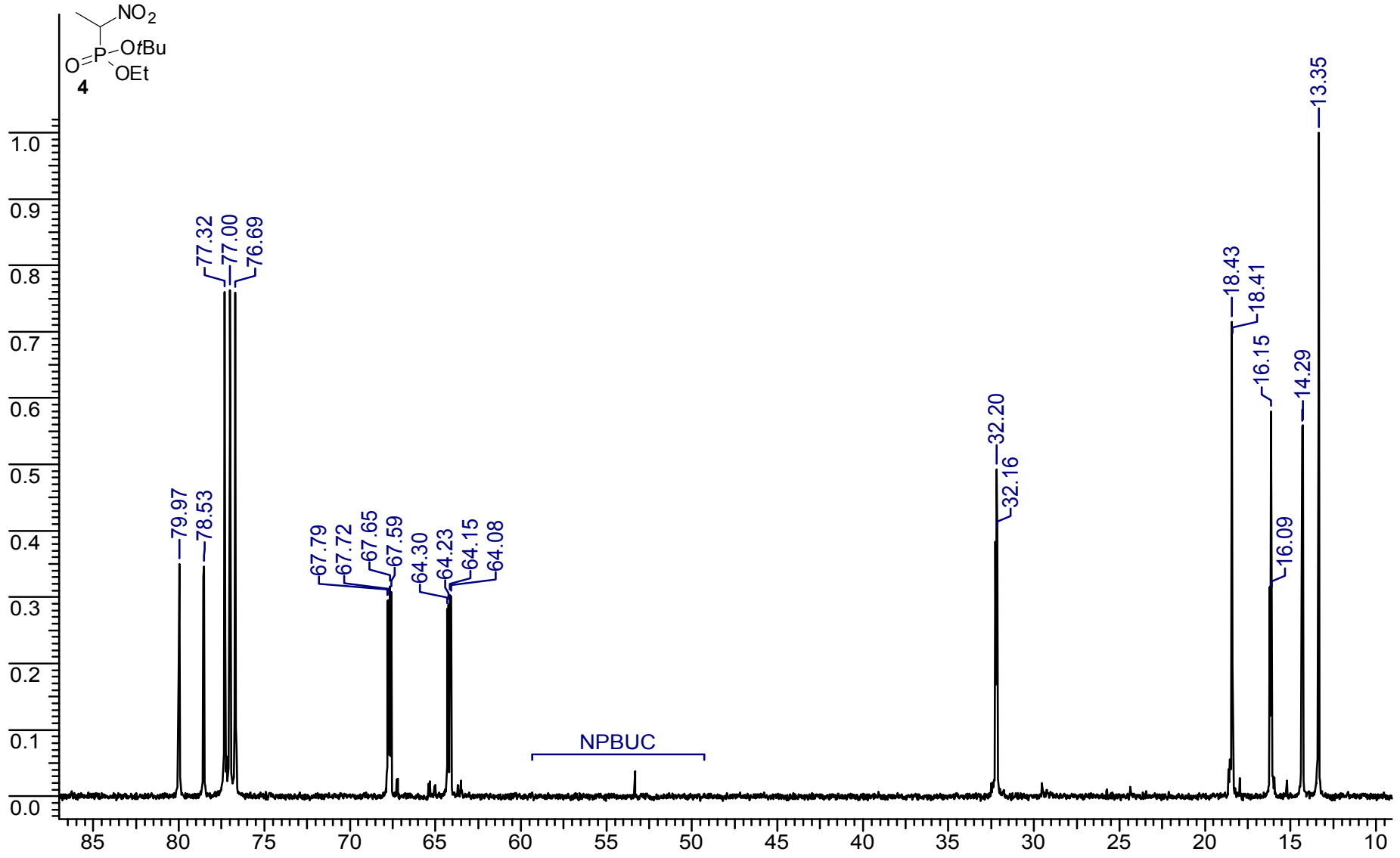
*^{31}P NMR (121.49 MHz) of compound **4***



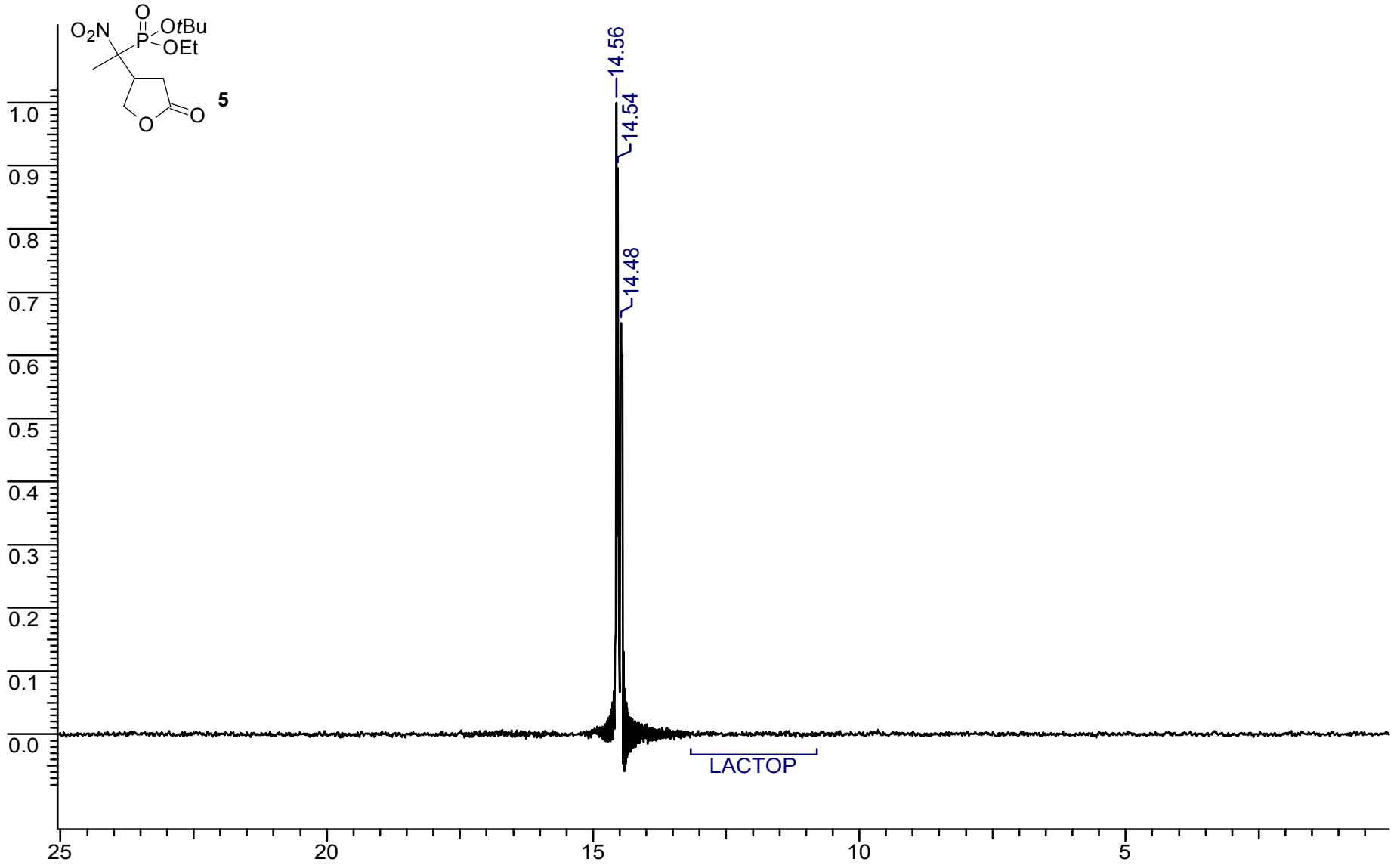
*^{1}H NMR (300.13 MHz) of compound **4***



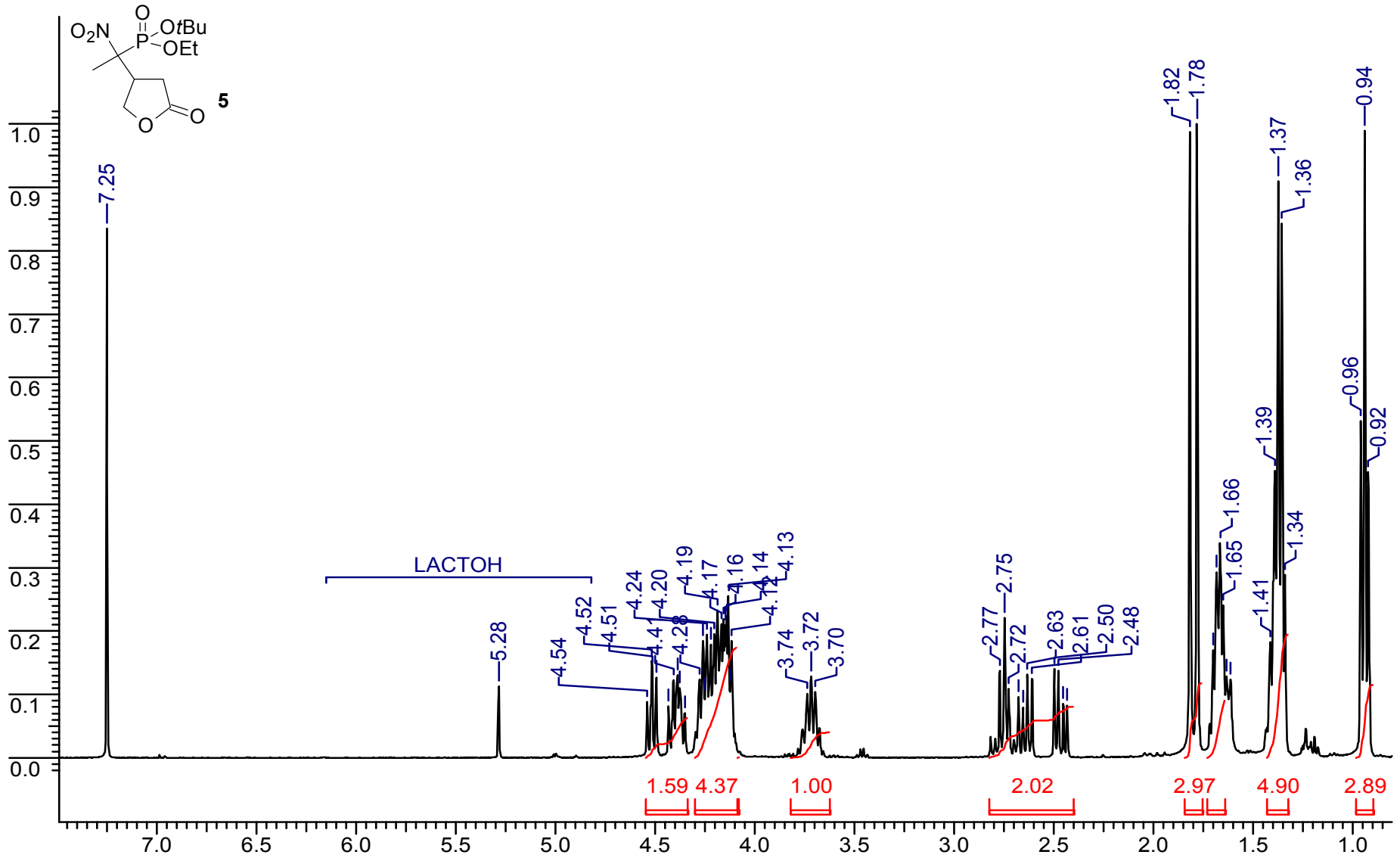
*^{13}C NMR (75.47 MHz) of compound **4***



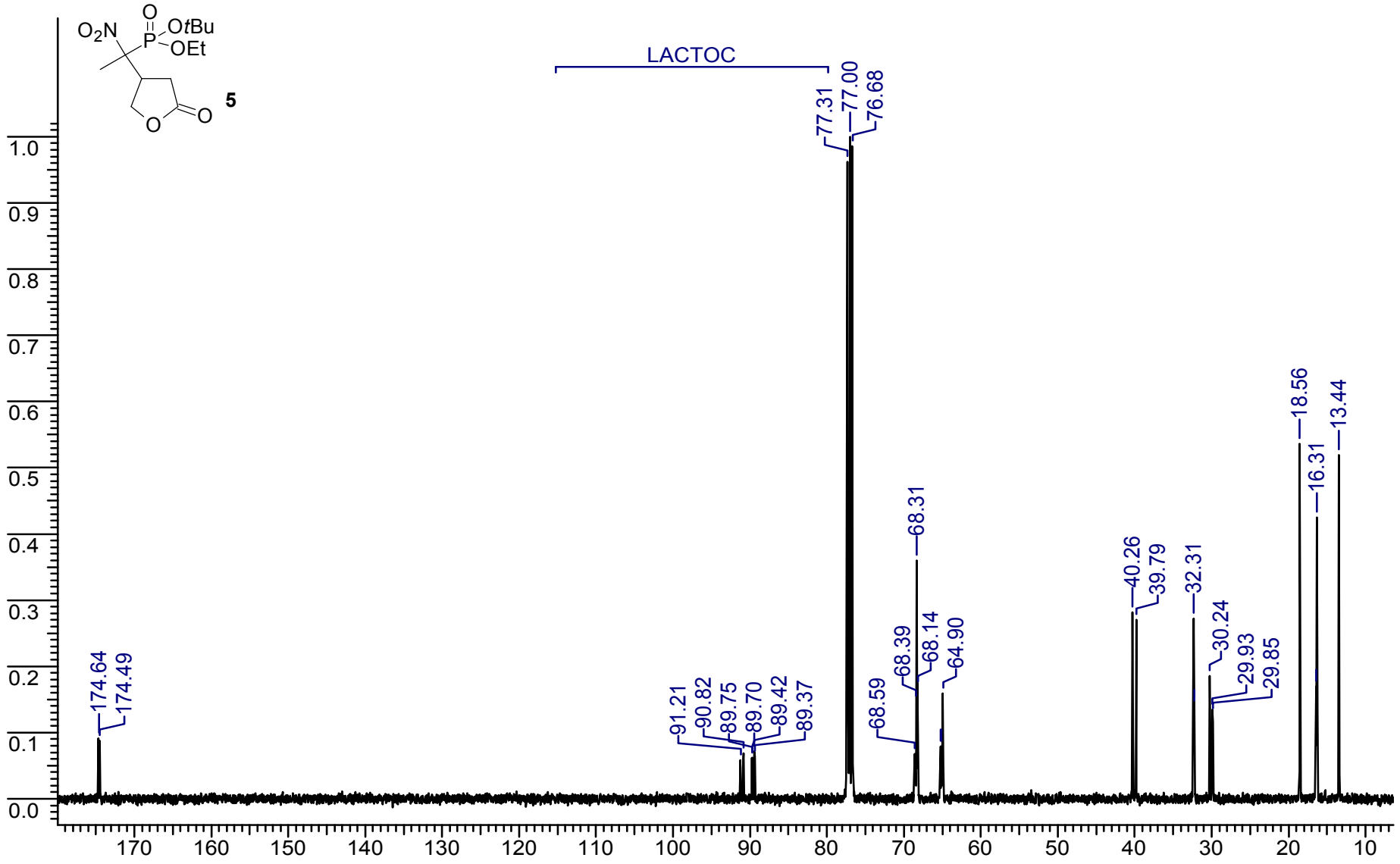
*^{31}P NMR (121.49 MHz) of compound **5***



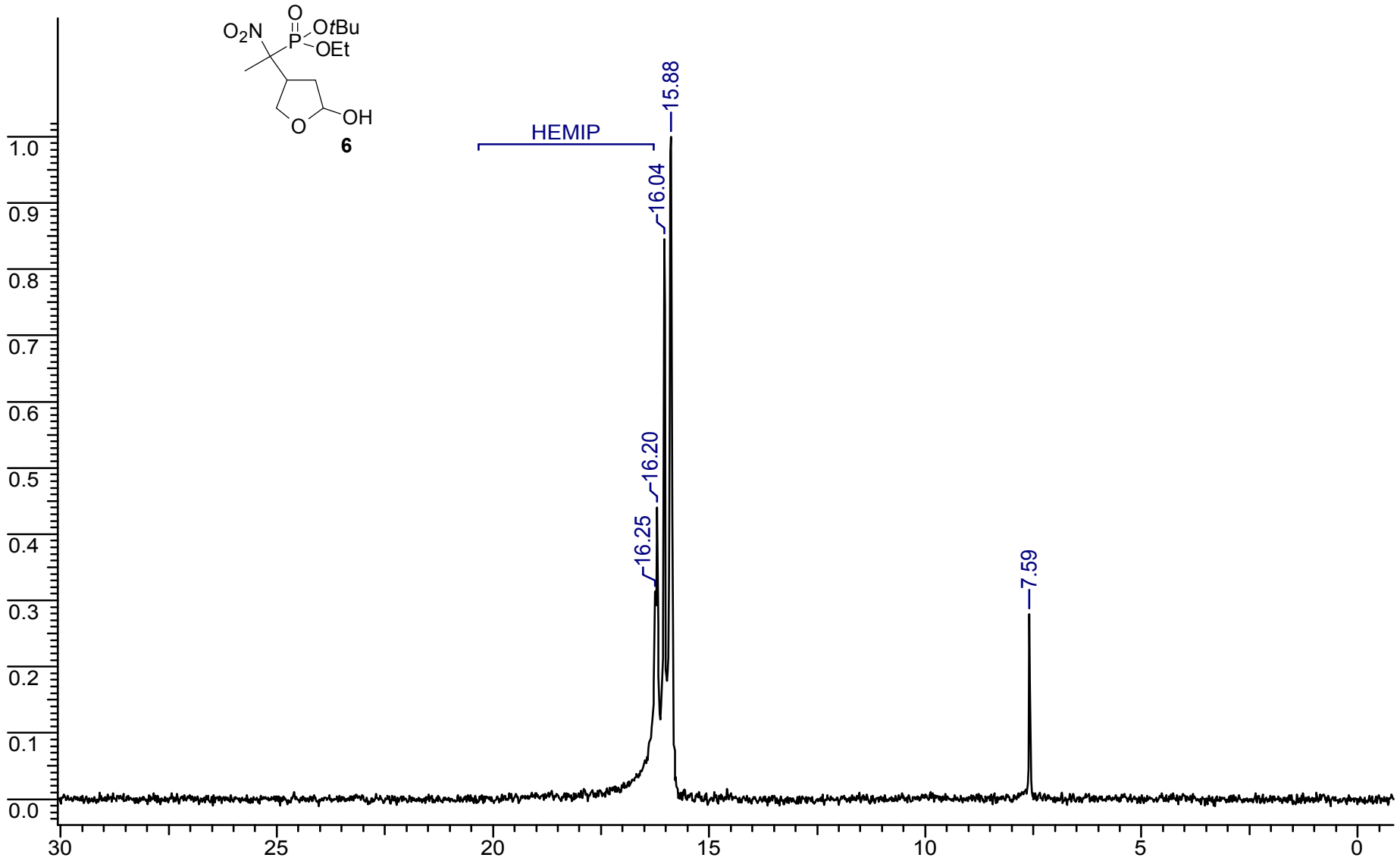
*^{1}H NMR (300.13 MHz) of compound **5***



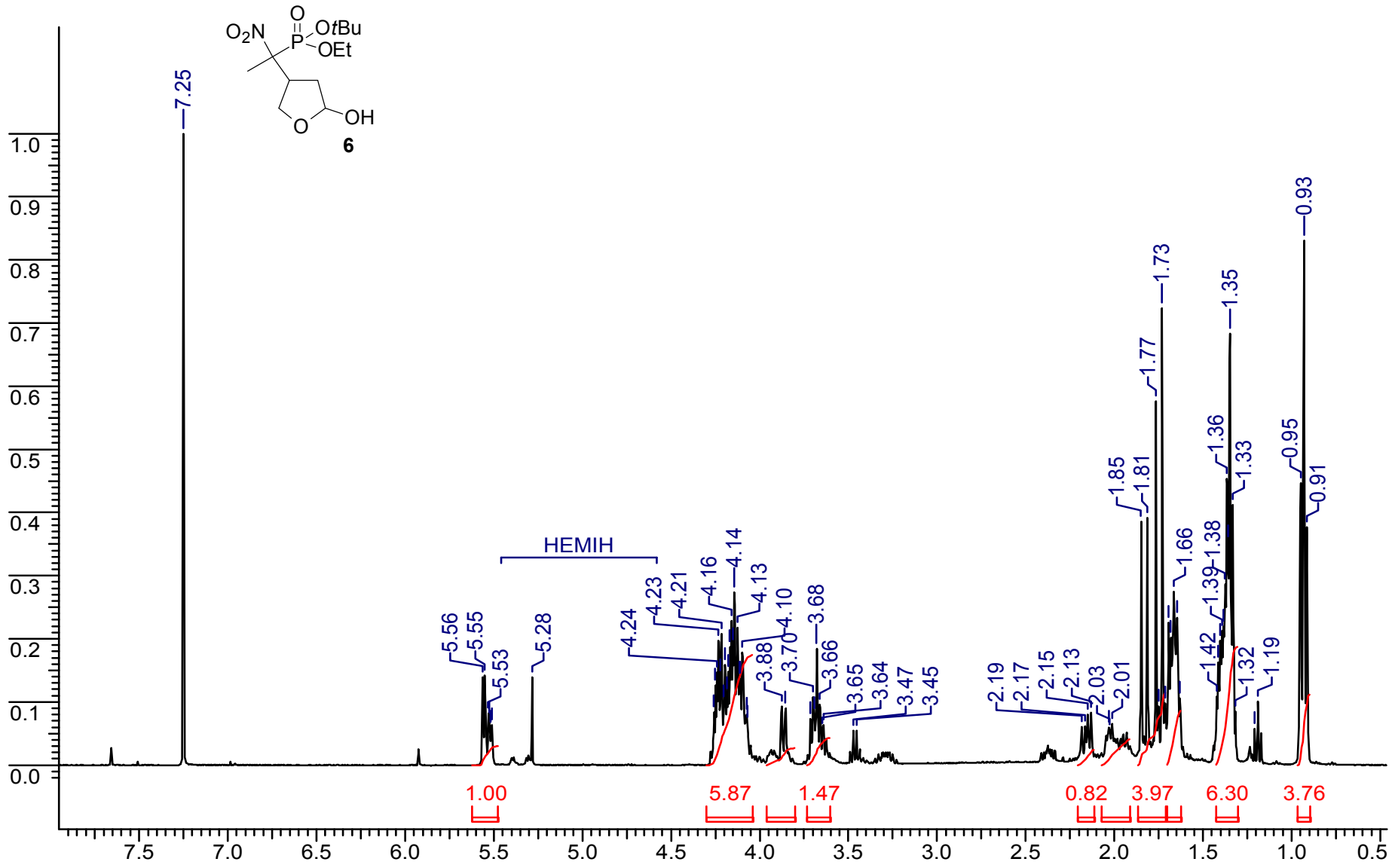
*^{13}C NMR (75.47 MHz) of compound **5***



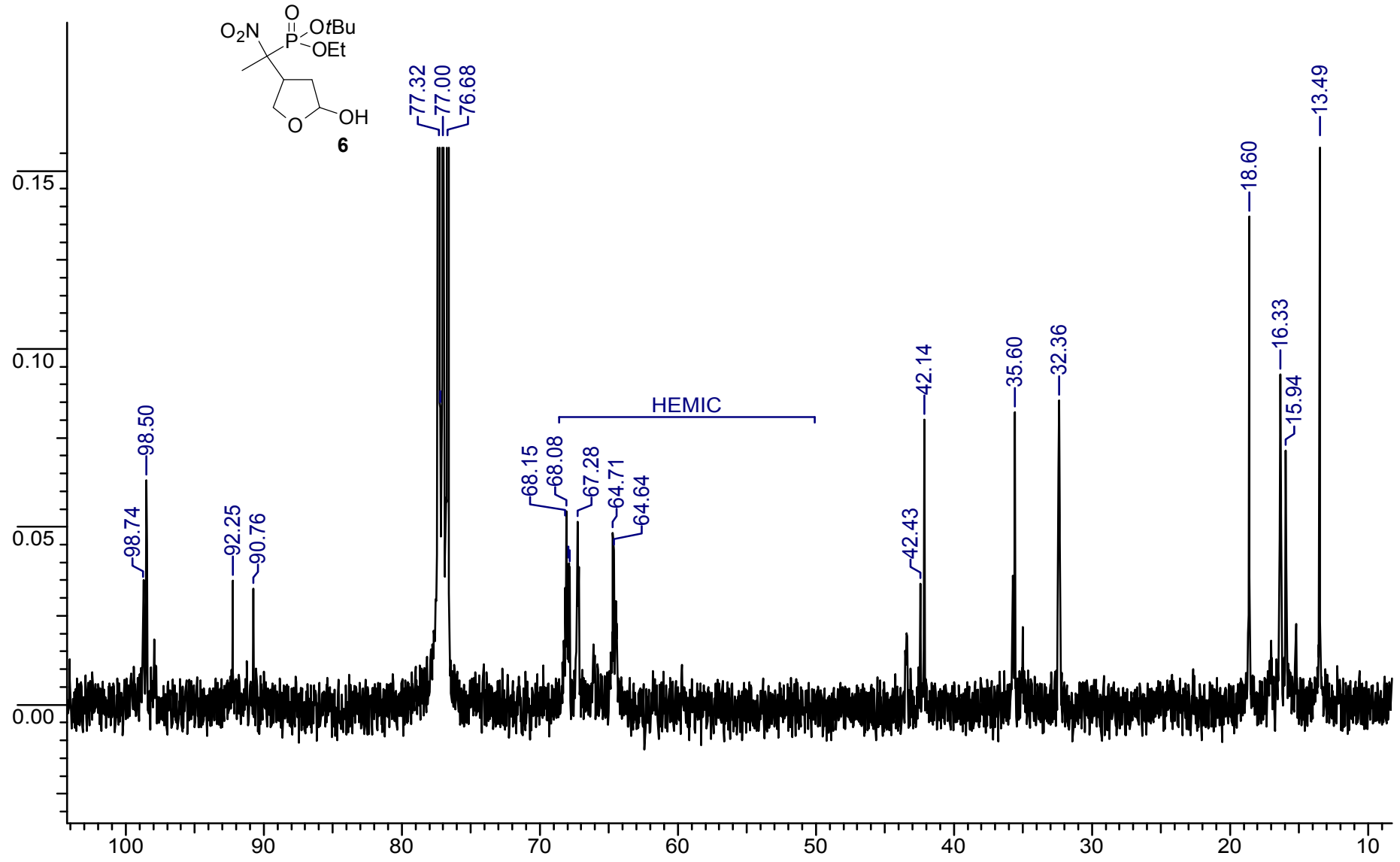
*^{31}P NMR (121.49 MHz) of compound **6***



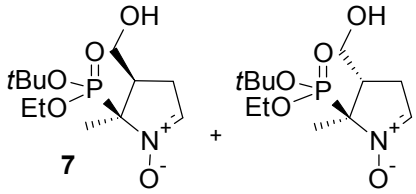
*^{1}H NMR (300.13 MHz) of compound **6***



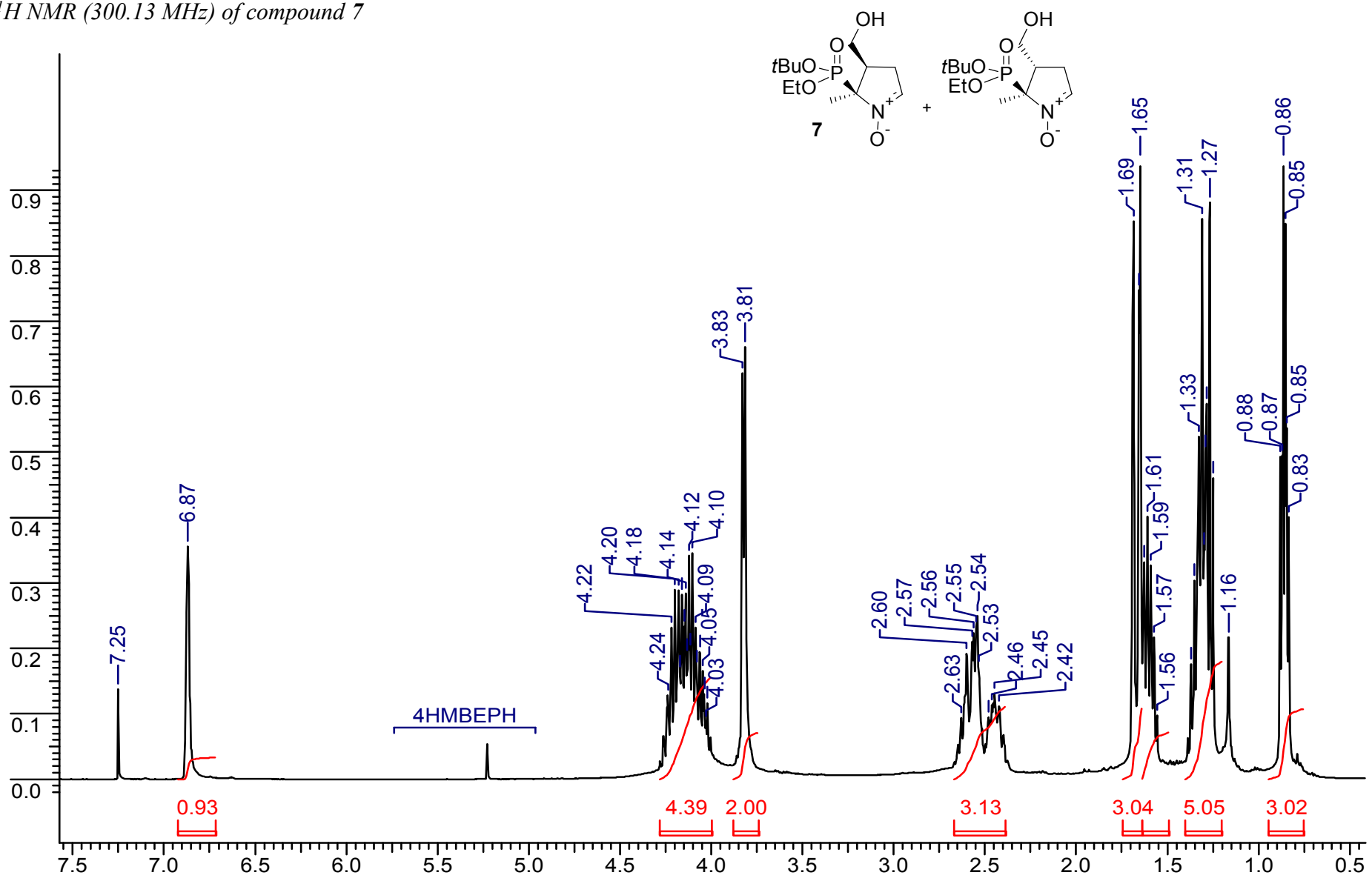
^{13}C NMR (75.47 MHz) of compound ***6***



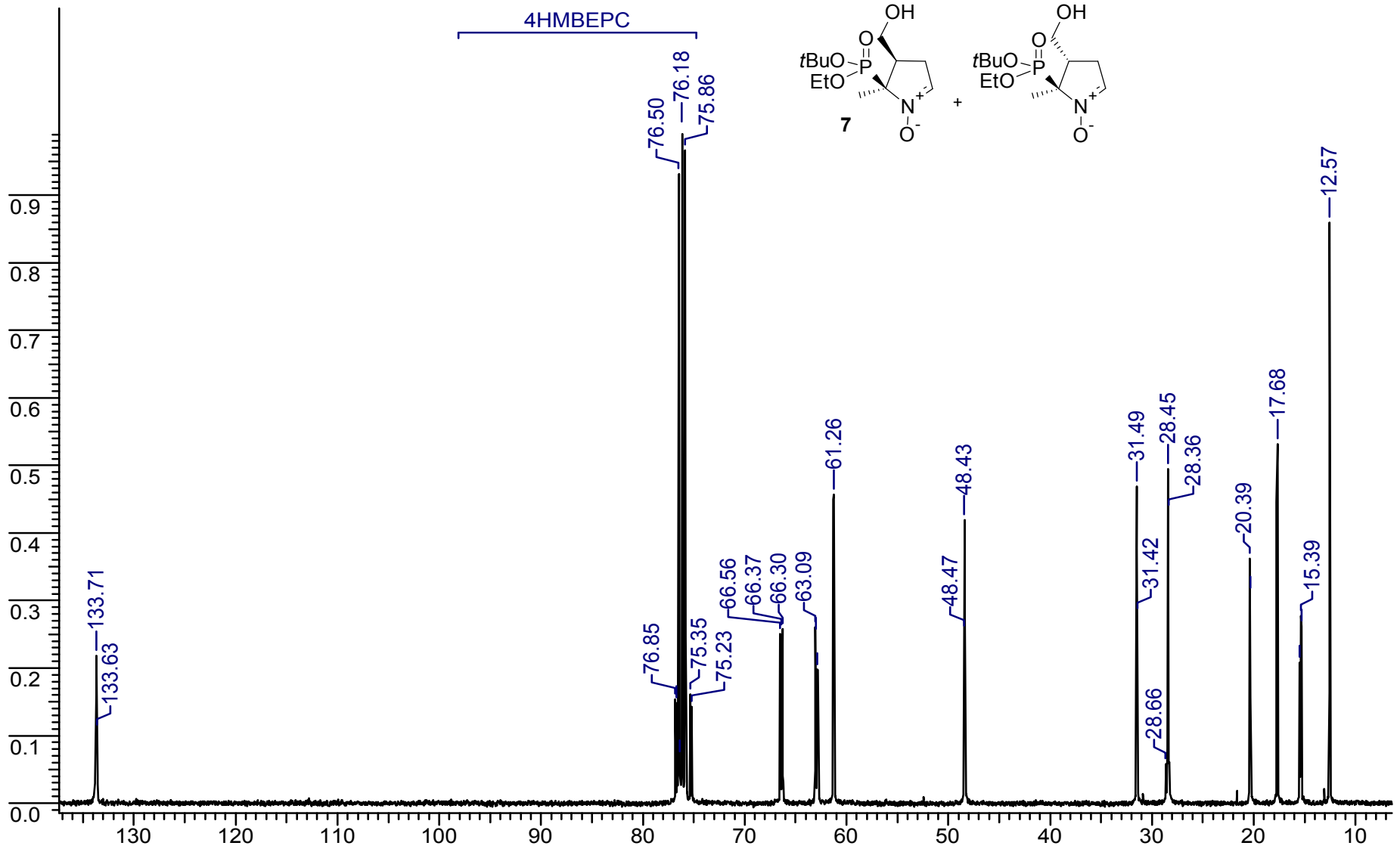
^{31}P NMR (121.49 MHz) of compound 7



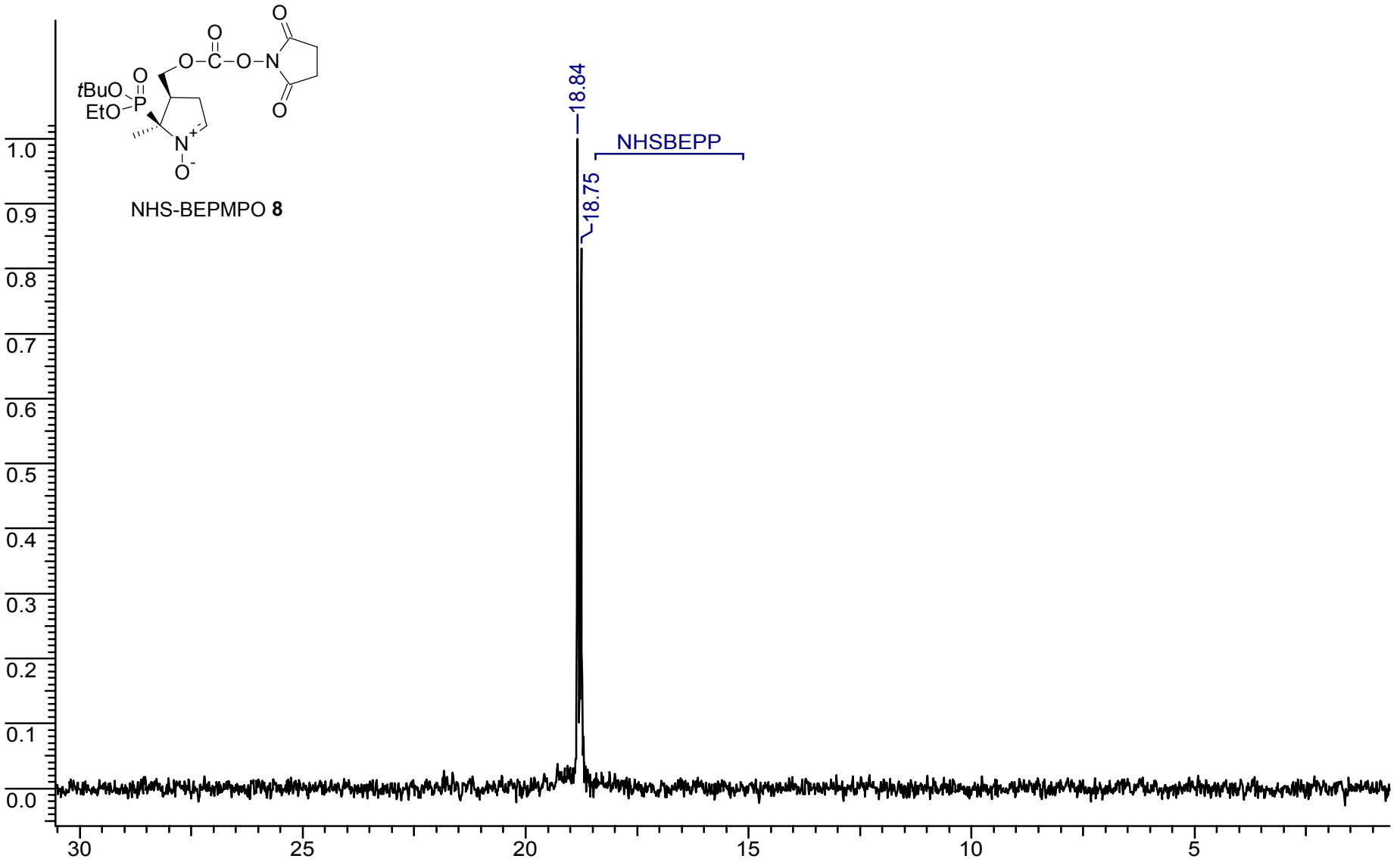
[1]H NMR (300.13 MHz) of compound 7



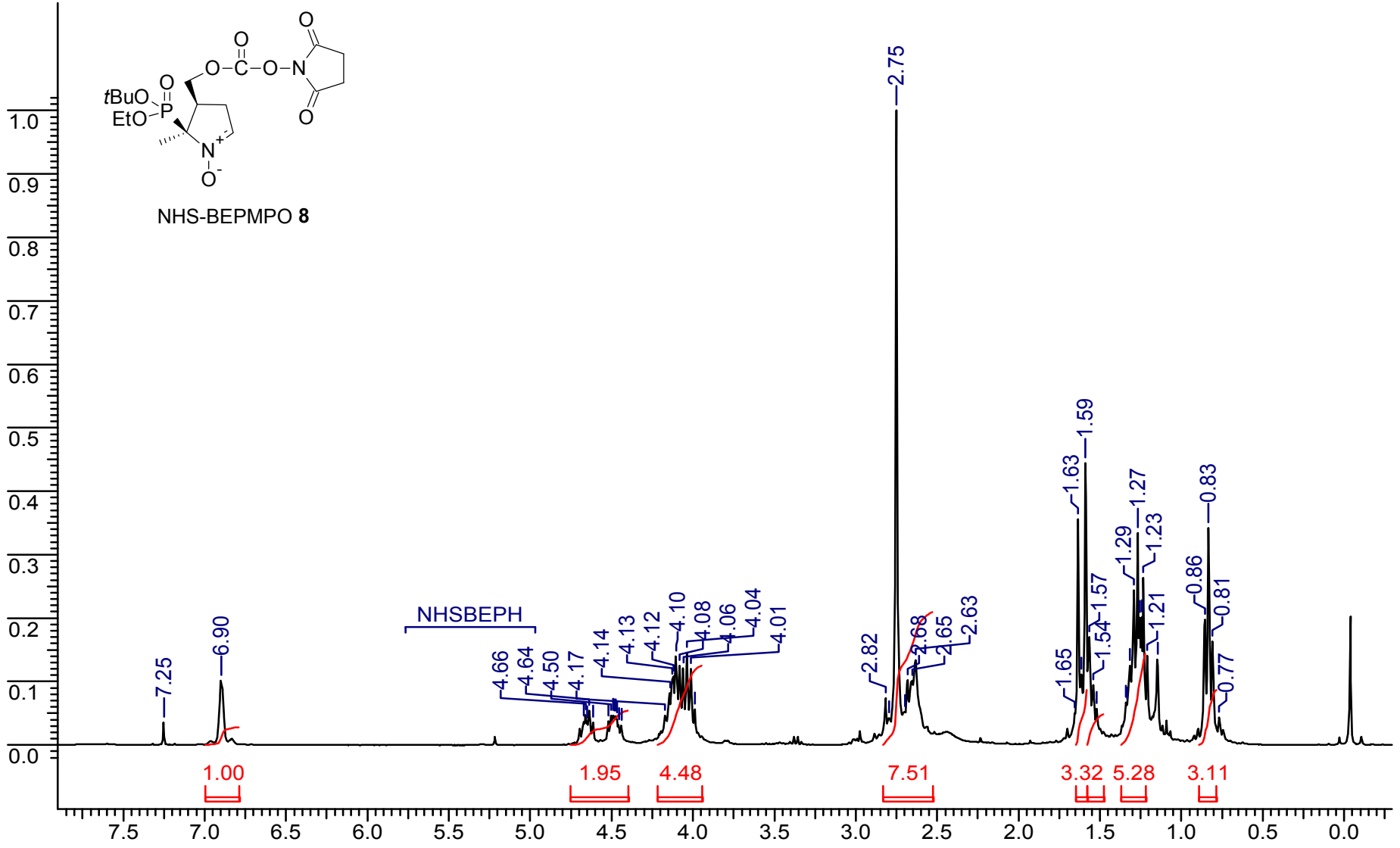
*^{13}C NMR (75.47 MHz) of compound **7***



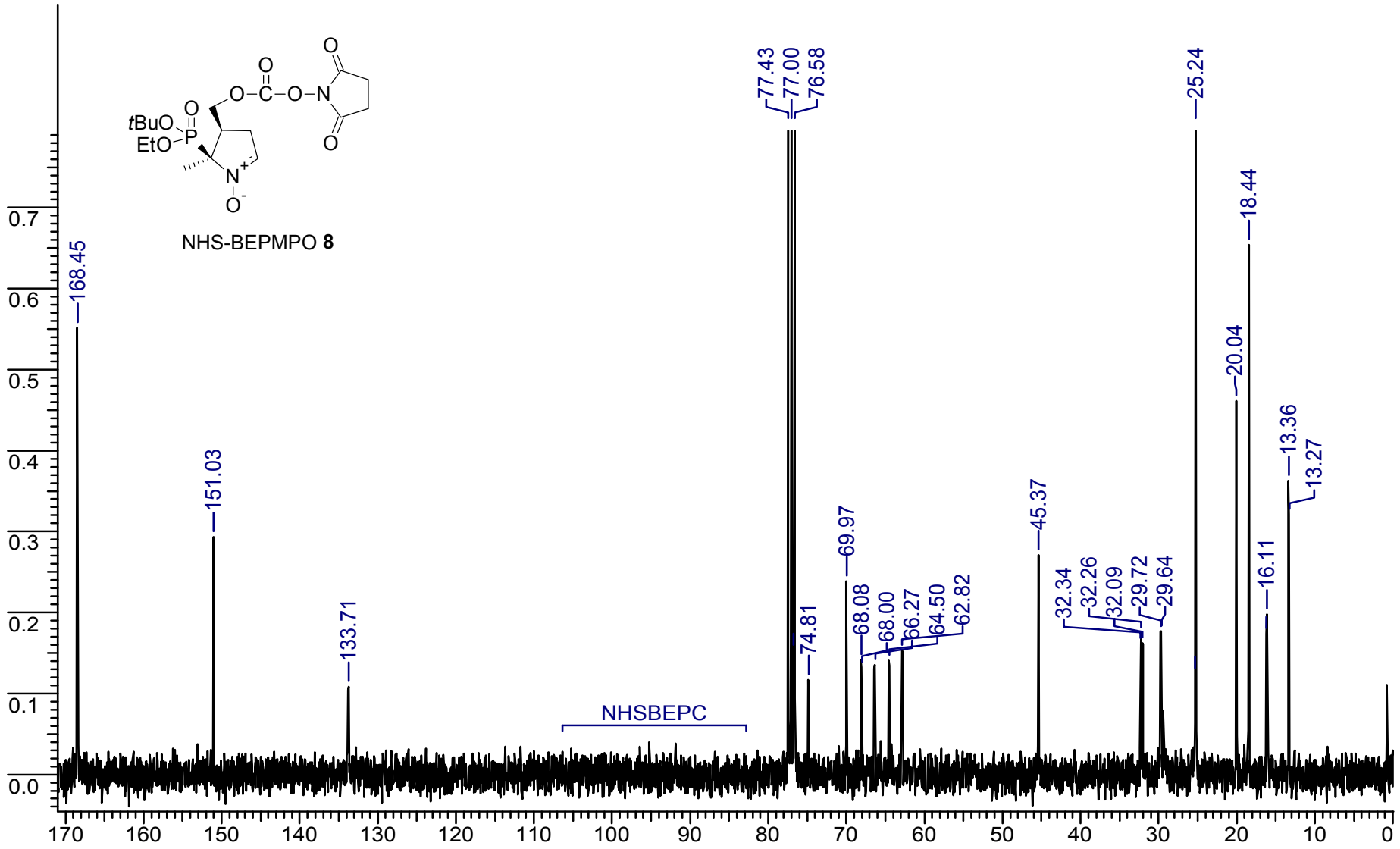
*^{31}P NMR (121.49 MHz) of compound **8***



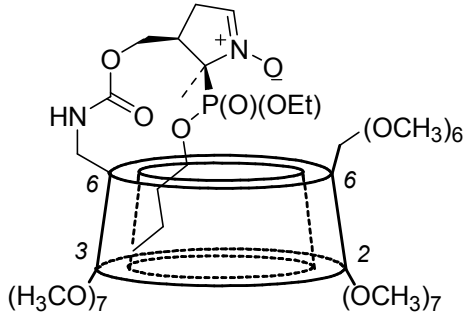
*[1]H NMR (300.13 MHz) of compound **8***



*^{13}C NMR (75.47 MHz) of compound **8***

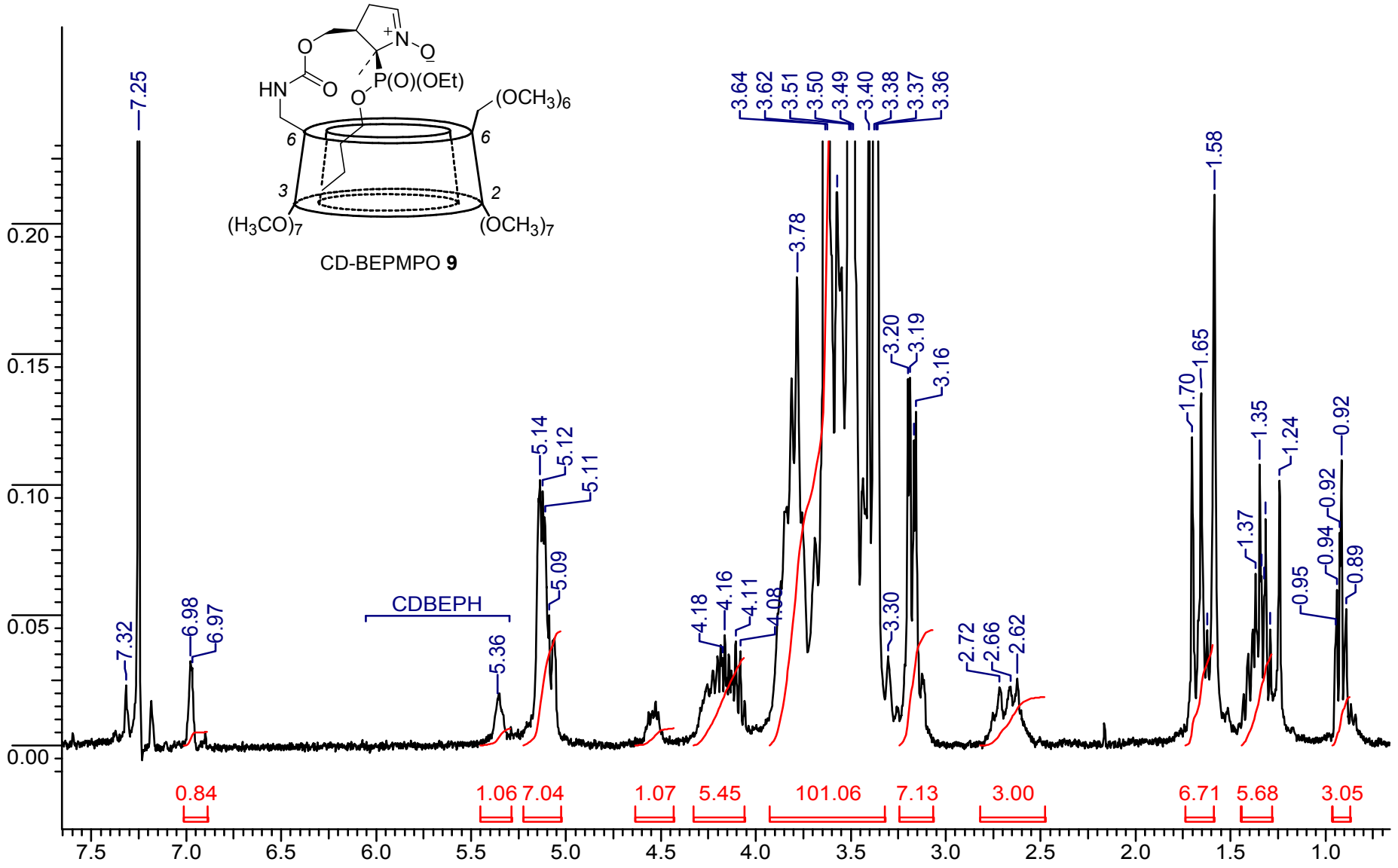


*^{31}P NMR (121.49 MHz) of compound **9***

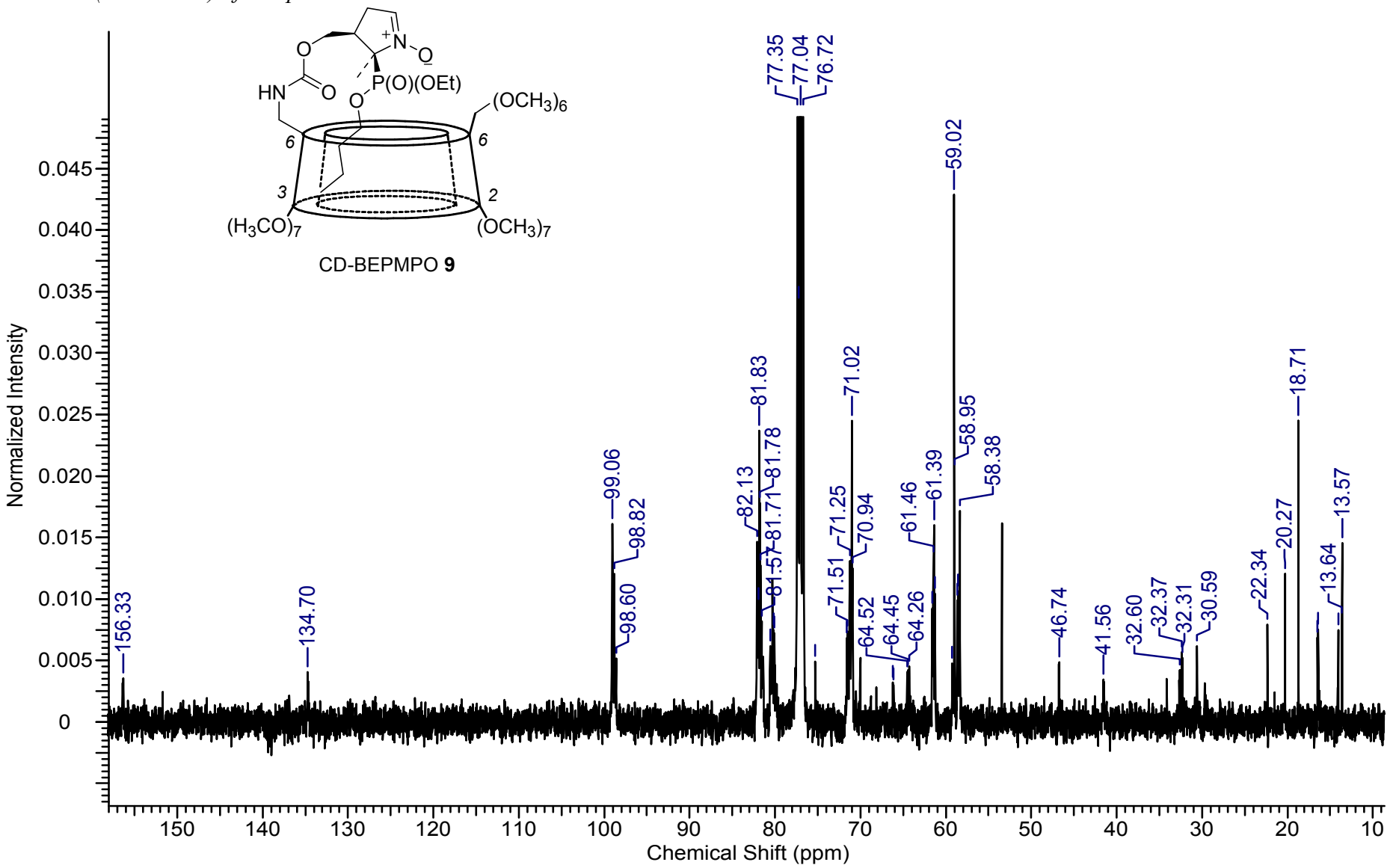


CD-BEPMPO **9**

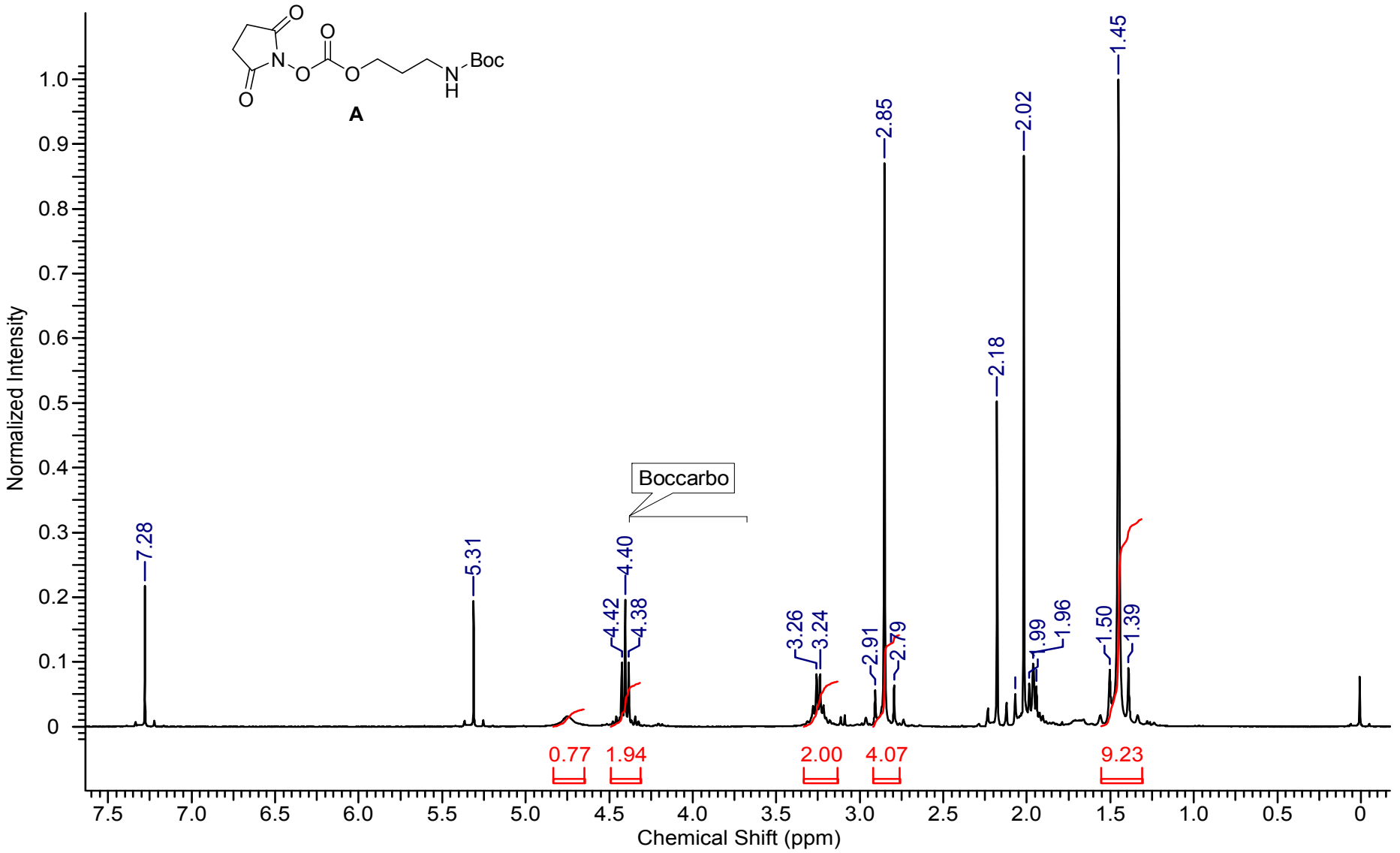
*[1]H NMR (300.13 MHz) of compound **9***



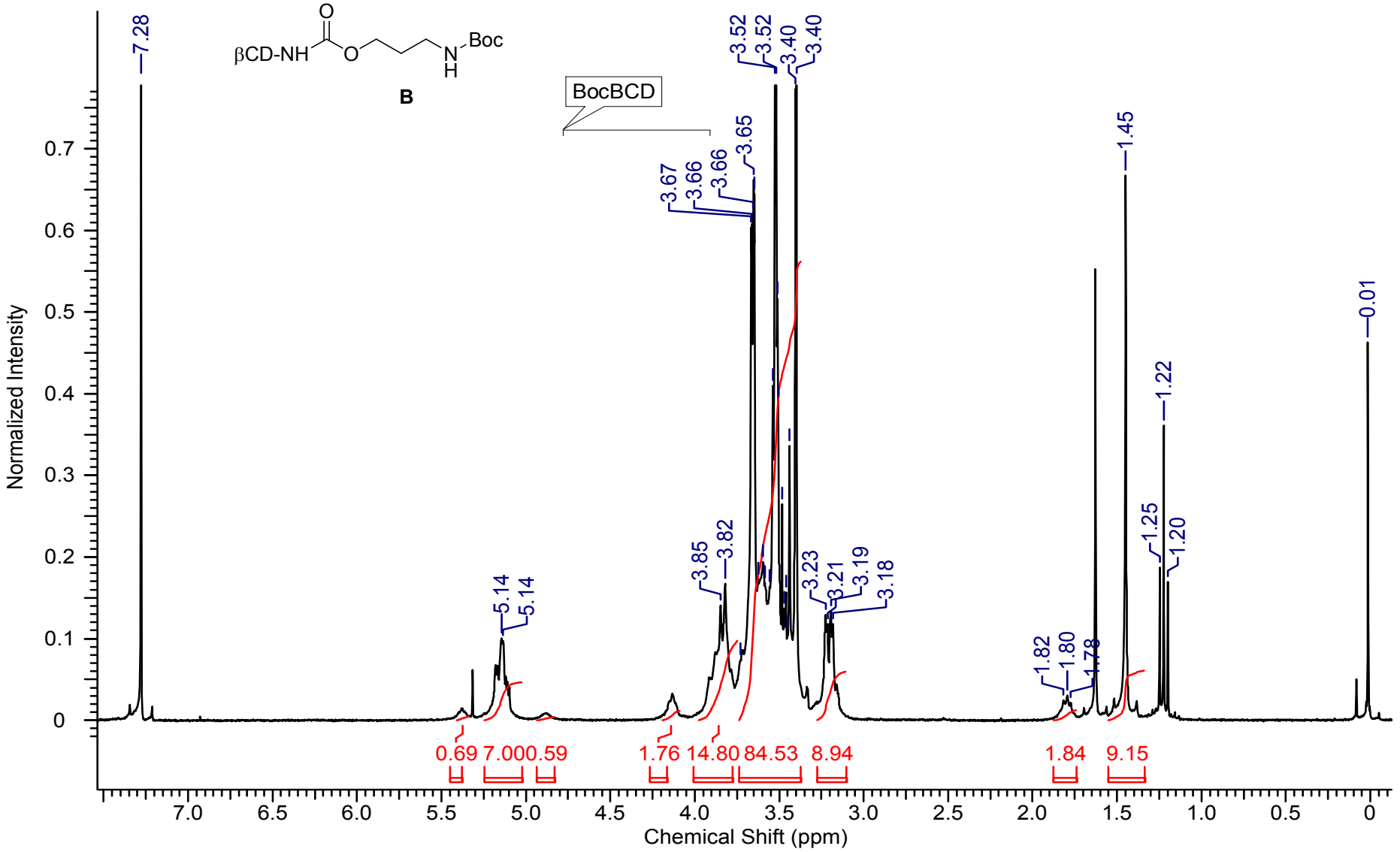
*^{13}C NMR (75.47 MHz) of compound **9***



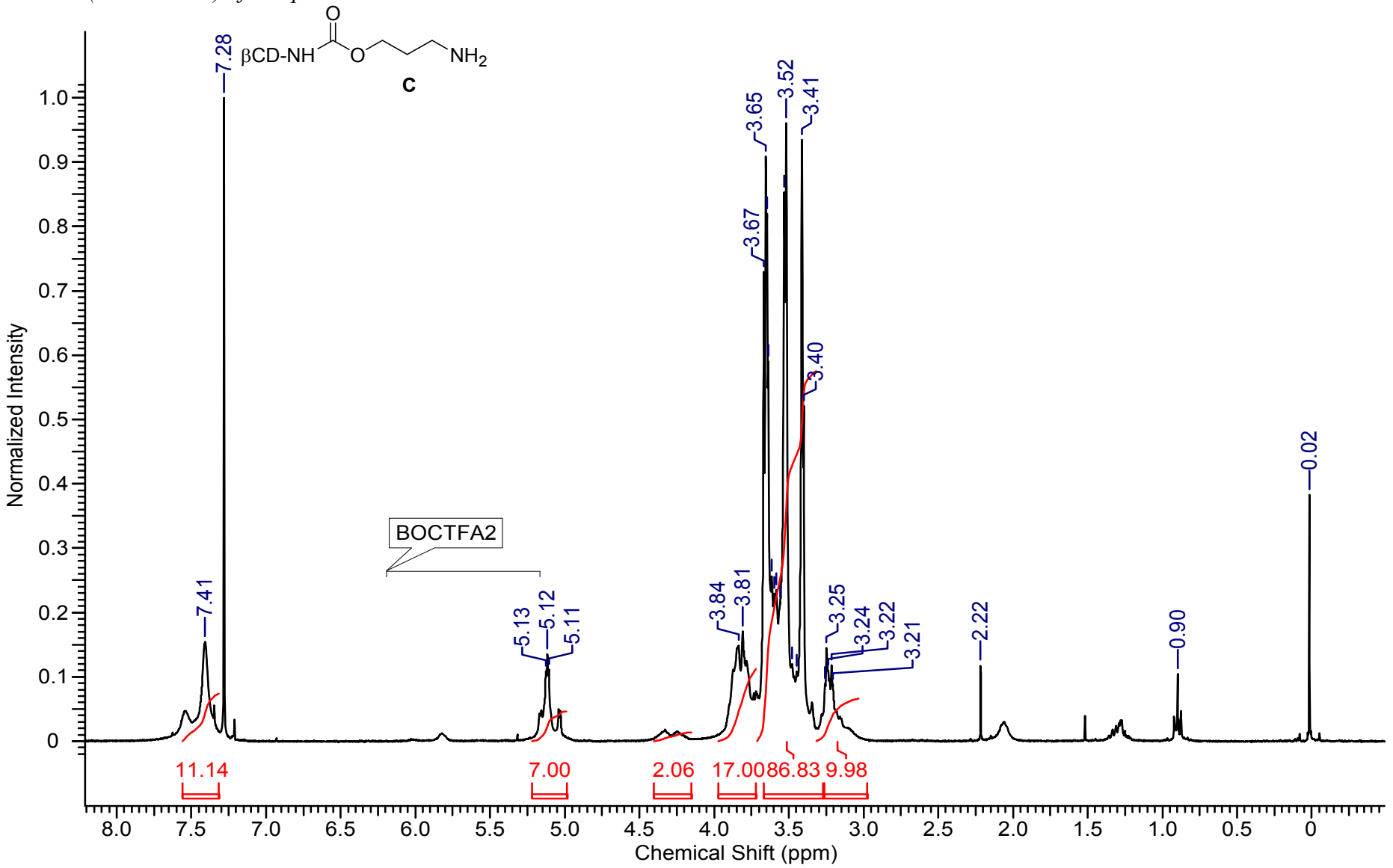
*^{1}H NMR (300.13 MHz) of compound **A***



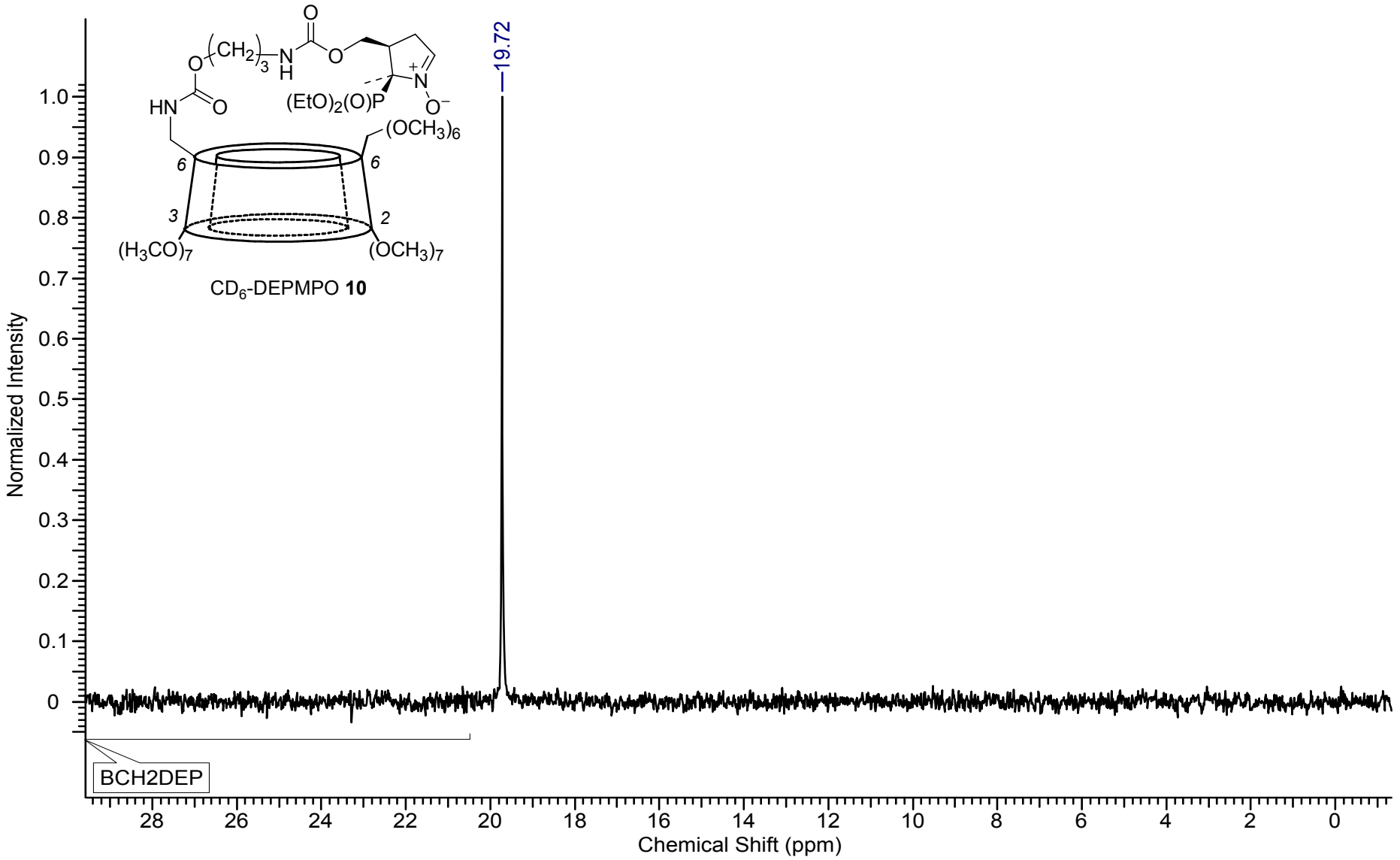
*[1]H NMR (300.13 MHz) of compound **B***



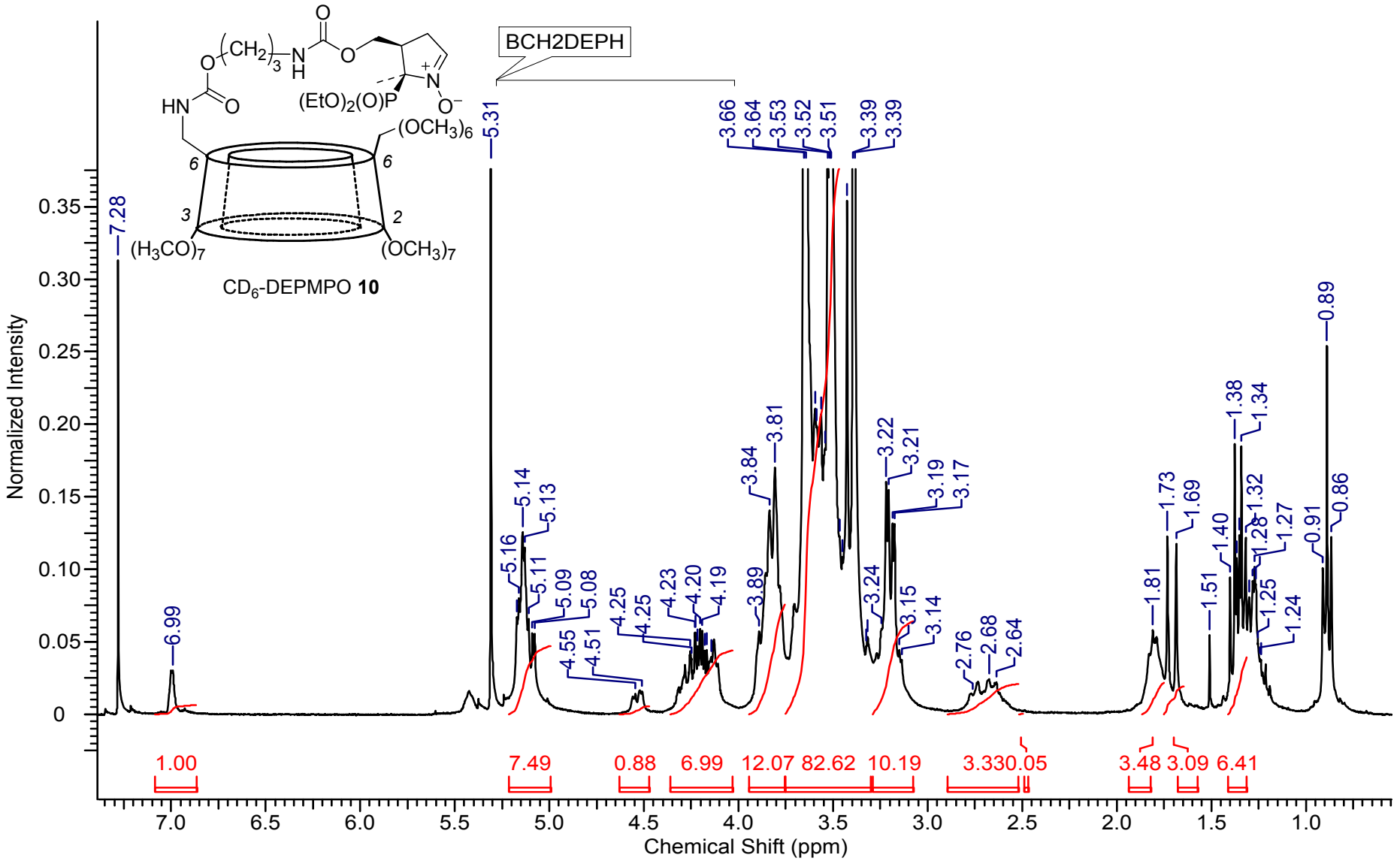
[1]H NMR (300.13 MHz) of compound ***C***



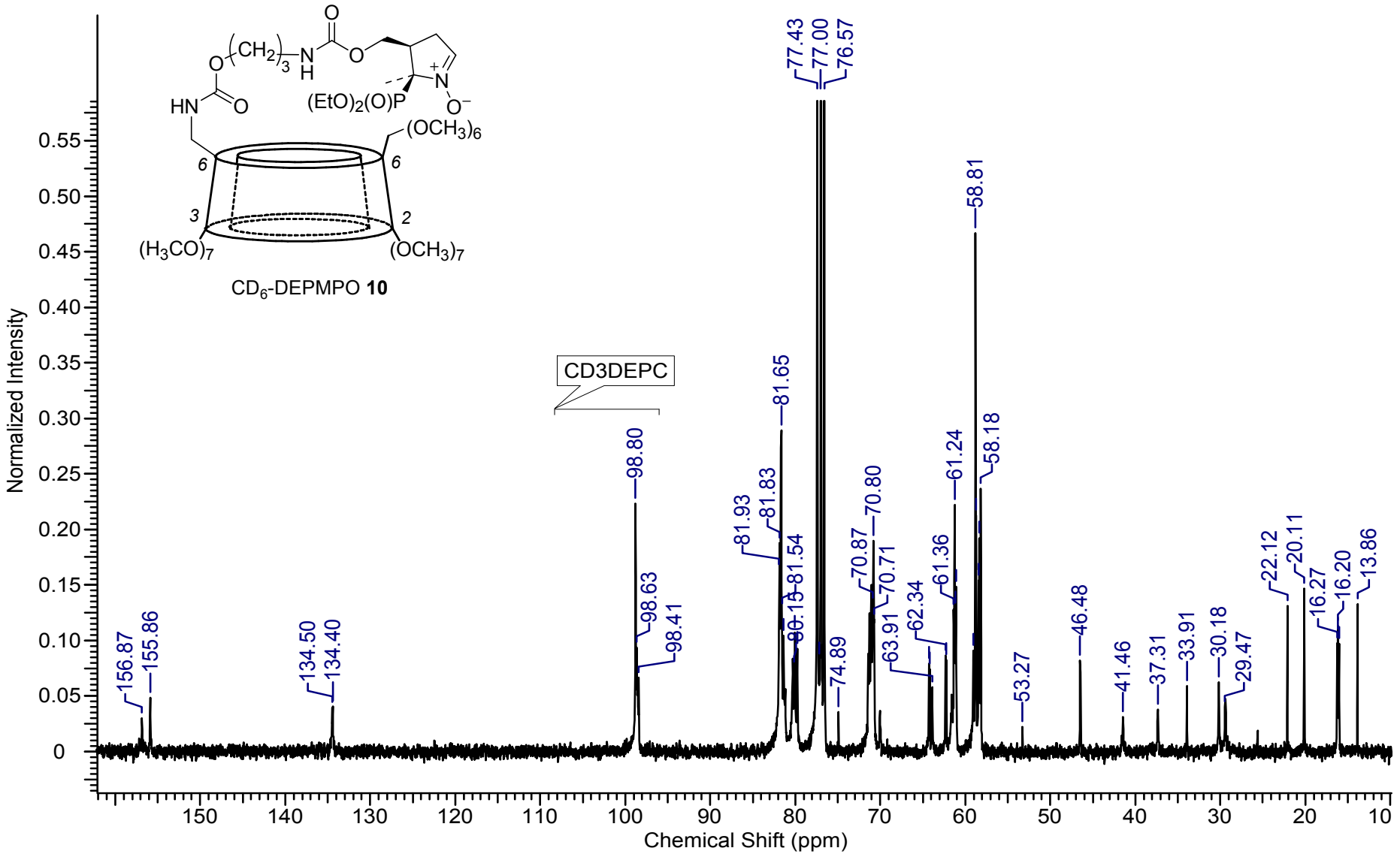
*^{31}P NMR (121.49 MHz) of compound **10***



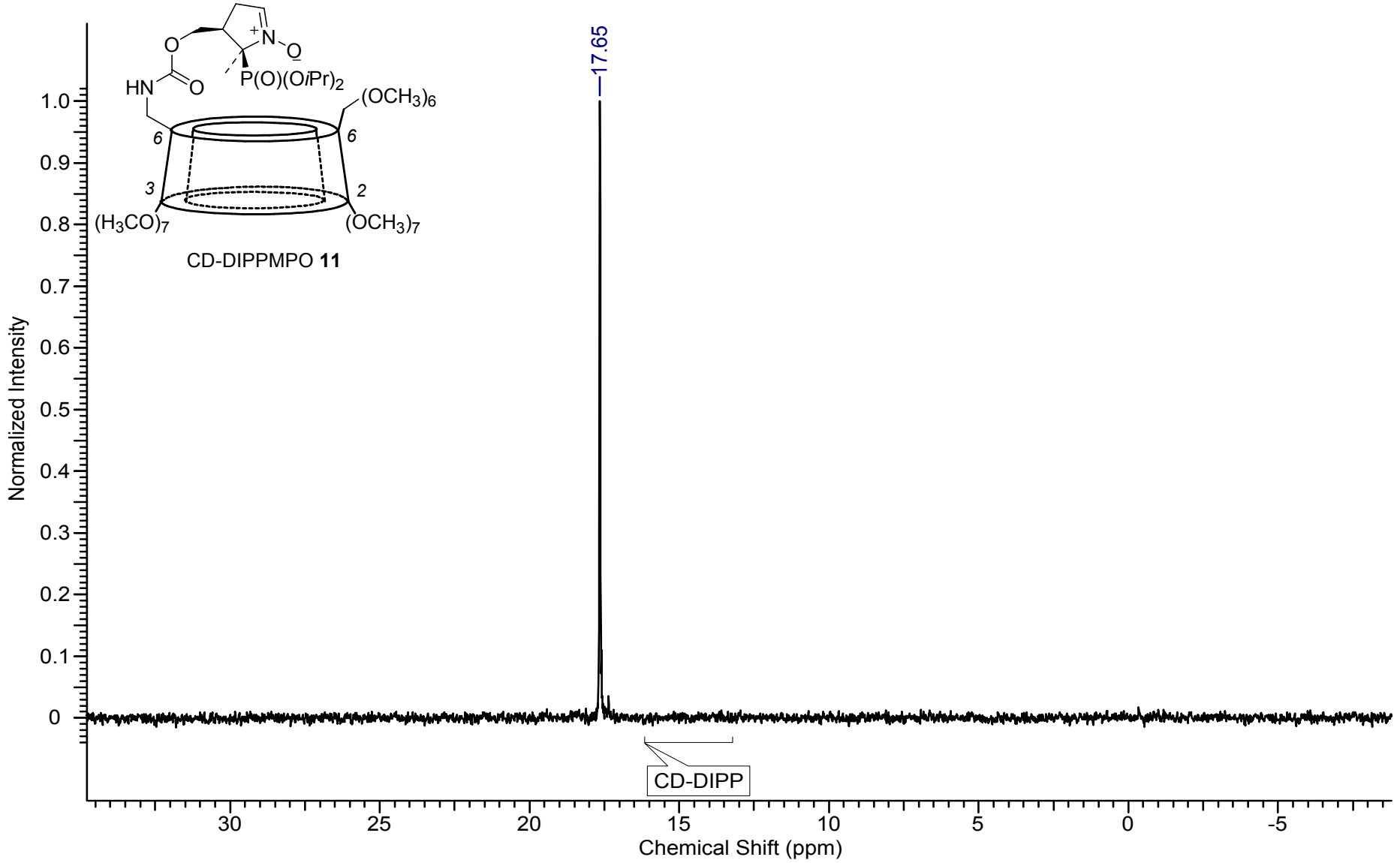
*^{1}H NMR (300.13 MHz) of compound **10***



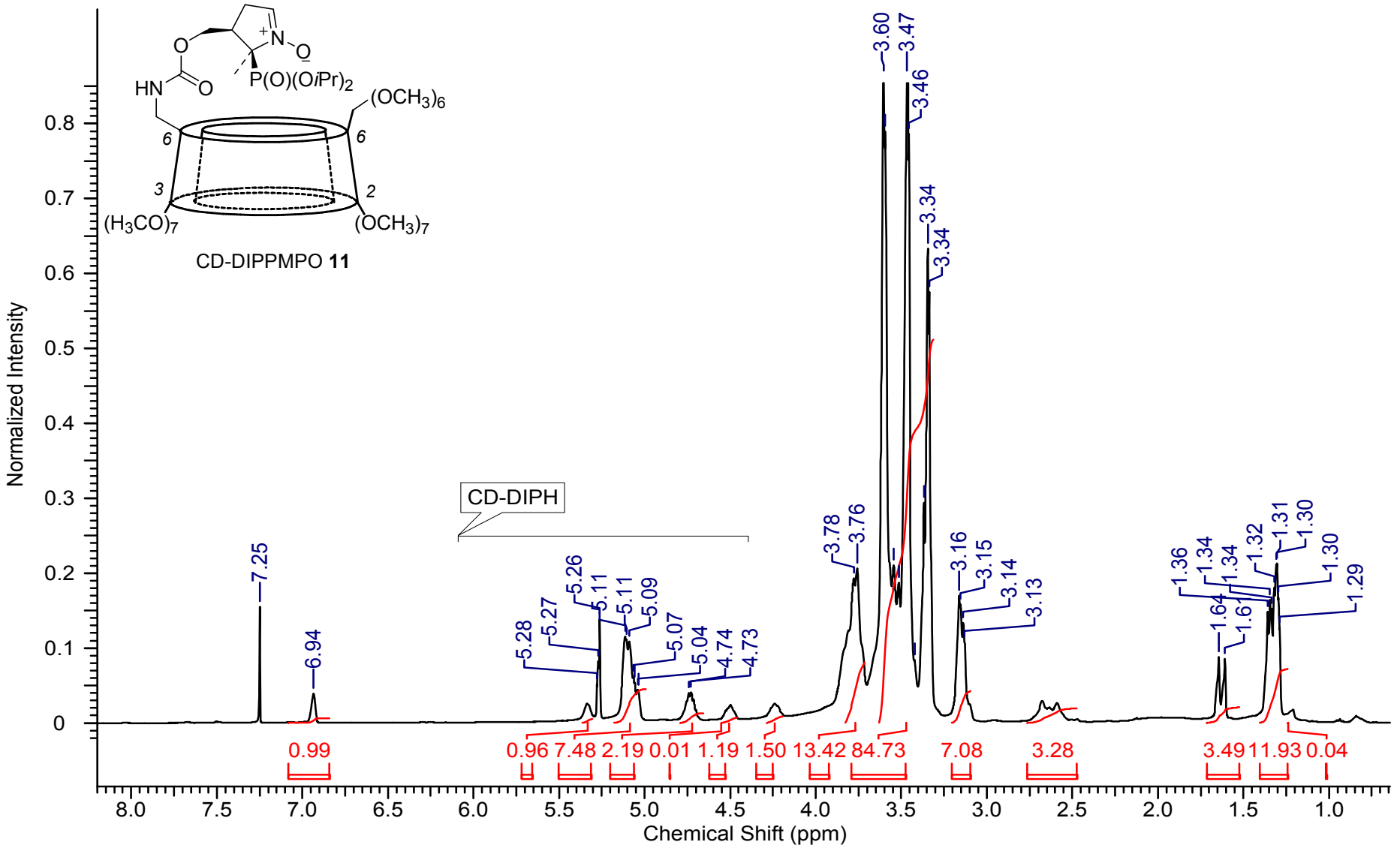
*^{13}C NMR (75.47 MHz) of compound **10***



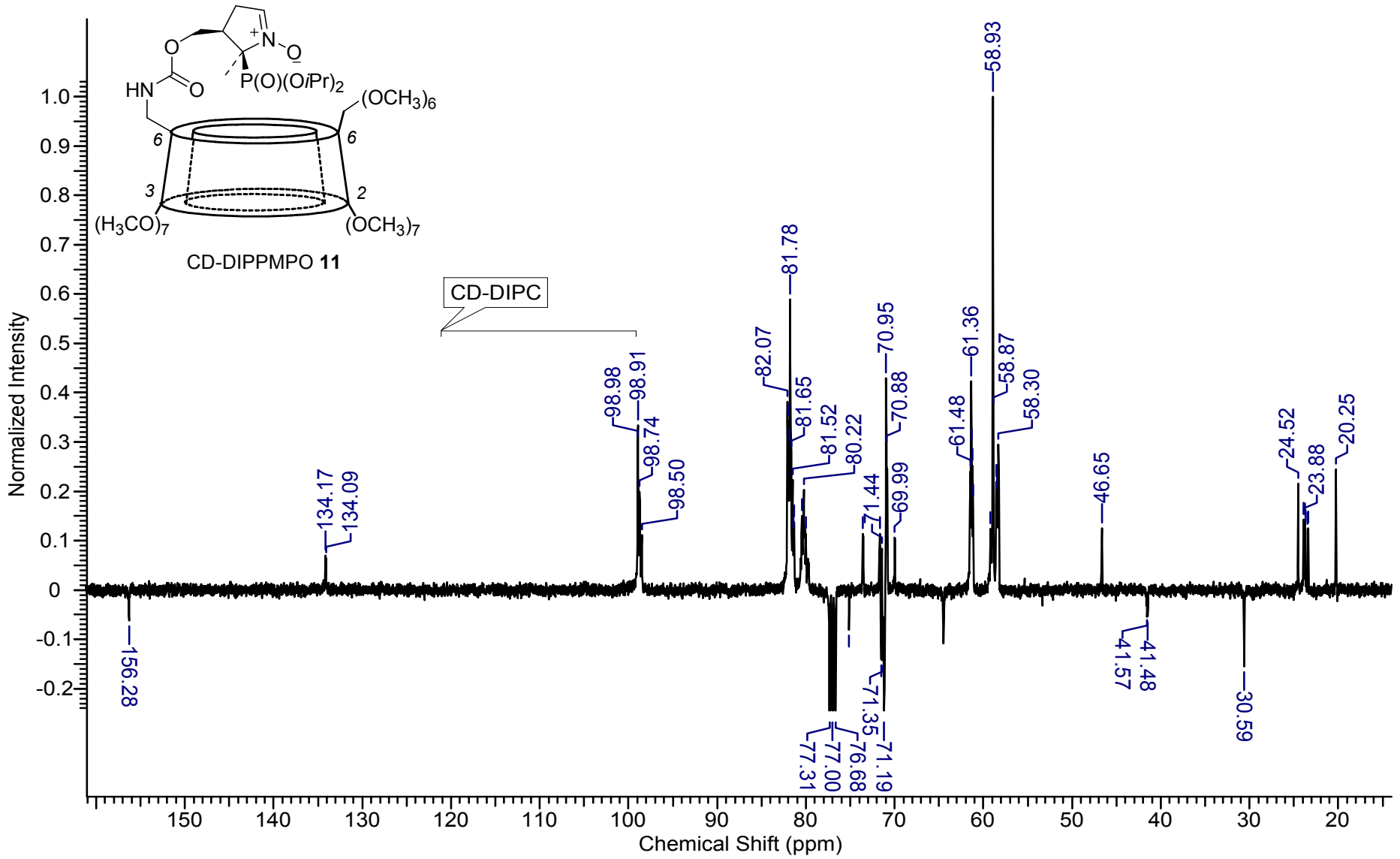
*^{31}P NMR (121.49 MHz) of compound **11***



*^{1}H NMR (300.13 MHz) of compound **11***



*^{13}C NMR (75.47 MHz) of compound **11***



MOLECULAR DYNAMICS SIMULATION

Molecular Dynamics (MD) calculations were performed with the Gromacs 5.1.2[3] package. Molecules were solvated in a quasi-cubic box which contained approximately 2000 water molecules. Concerning the force fields used in the MD simulations, we used the TIP3P[4] force field to describe the water molecules, the AMBER force field (ff99SB)[5] including additional parameters for nitroxide moieties developed by Barone *et al.*[6] and the atomic charges were computed at the HF/6-31G(d) level of theory with the RESP scheme.[7] In order to optimize the simulation box size, we performed a NPT calculation at 300K and 1 bar during 300 ps with a time step of 2.5 fs. After this first stage, we performed a NVT trajectory at 300K during 50 ns with a time step of 2.5 fs. We kept the last 49.5 ns of the two trajectories for the data analysis calculations.

Table S1: Parameters used for the simulation of the spectra in Fig. S1.

Spin trap	Spin adduct	Conformer	Exchange time	A_P (mT)	A_N (mT)	A_{Hb} (mT)	AP_{Hg} (mT)
BMPO	BMPO-OH (100 %)	-	-	-	1.41	1.27	-
DEPMPO	DEPMPO-OOH *trans* (20 %)	T1 (53 %)	32 ns	5.19	1.31	1.19	0.08
		T2 (47 %)		4.85	1.32	1.01	0.09
	DEPMPO-OH (80 %)	-		4.71	1.40	1.32	-
DIPPMPO	DIPPMPO-OH (100 %)	-	-	4.68	1.40	1.33	-
Mito-DIPPMPO	Mito-DIPPMPO-OOH *trans* (75 %)	T1 (52 %)	41 ns	5.33	1.28	1.48	-
		T2 (48 %)		5.29	1.29	0.87	-
	Mito-DIPPMPO-OH (25 %)	-	-	5.29	1.36	1.05	-
CD-DIPPMPO	CD-DIPPMPO-OOH *trans* (100 %)	T1 (54 %)	64µs	5.34	1.26	1.25	-
		T2 (46 %)		5.26	1.30	1.12	-

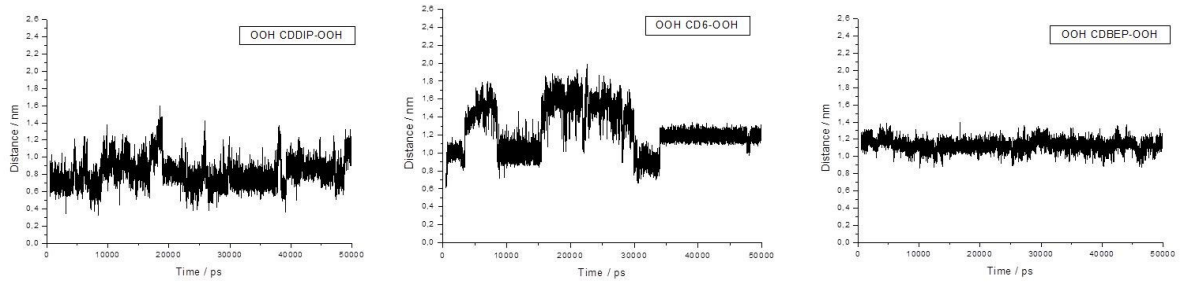


FIG. S1. Time evolution of the distances

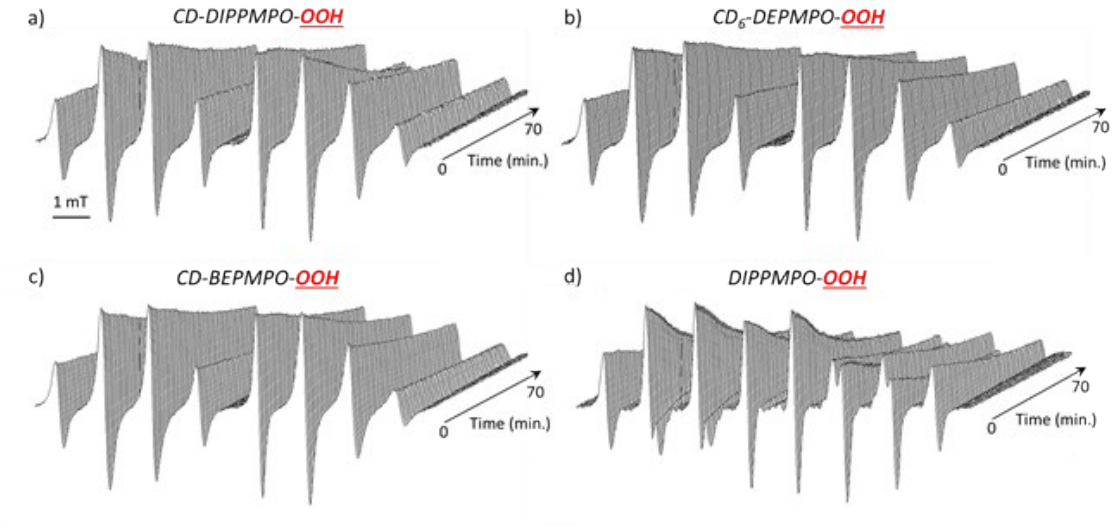


FIG. S2. Experimentals spectra of the kinetics of decay. a) CD-DIPPMPO-OOH (**11**-OOH), b) CD_6-DEPMPO-OOH (**10**-OOH), c) CD-BEPMPO-OOH (**9**-OOH) and d) DIPPMPO-OOH. Kinetics of decay of spin adducts generated by HX (0.4 mM), XO (0.04 U mL^{-1}), DTPA (1 mM) in an oxygenated phosphate buffer (0.1 M, pH 7.4), and addition of SOD (600 $U.mL^{-1}$).

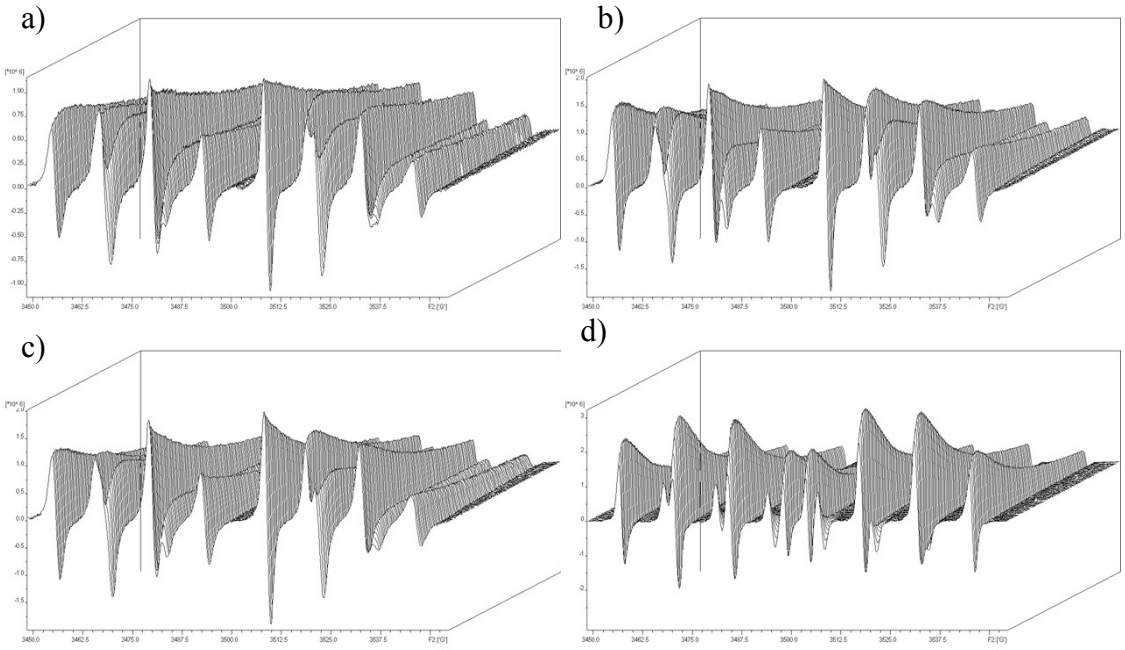


FIG. S3. Decay kinetics of superoxide adducts in the presence of GSH (a) Decay kinetics of superoxide spin adducts generated by HX (0.4 mM), XO (0.04 U mL^{-1}), DTPA (1 mM) in an oxygenated phosphate buffer (0.1 M, pH 7.4), and addition of SOD (600 $U.mL^{-1}$), GSH (1 mM) in the presence of CD-DIPPMPO (20 mM). (b) as in (a) with CD_6-DIPPMPO. (c) as in (a) with CD-BEPMPO. (d) as in (a) with DIPPMPO.

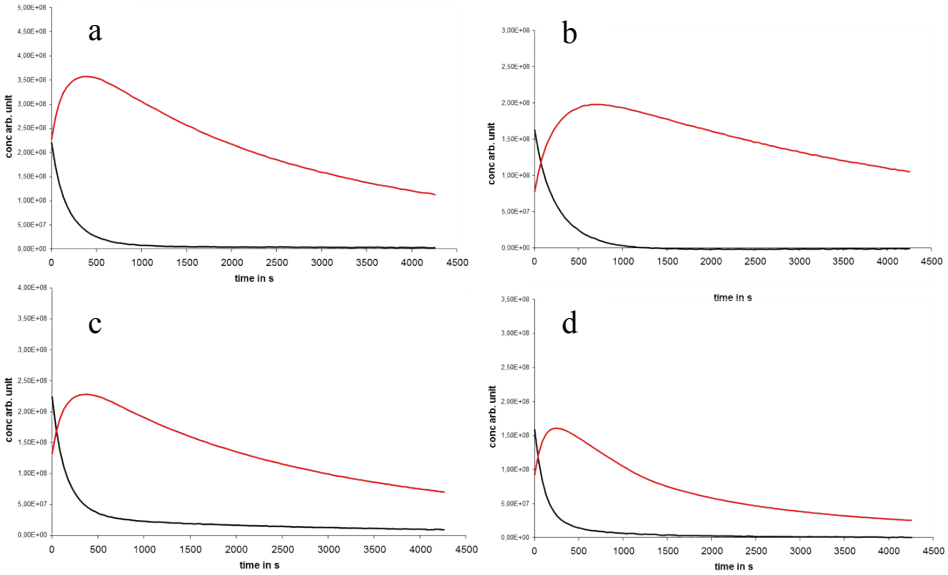


Figure S4. Effects of Glutathione on the superoxide adducts (black line: EPR signal intensity of superoxide adduct; red line: hydroxyl adduct)a) CD-BEPMPO, b) CD-DIPPMPO, c) CD6-DIPPMPO, d) DIPPMPO.

Adducts-OOH	$t_{1/2}$ (min.)
CD-BEPMPO-OOH	2.5
CD_6-DEPMPO-OOH	3
CD-DIPPMPO-OOH	3.5
DIPMPO-OOH	1.8

Table S2. Persistency of the superoxide adducts in the presence of GSH (1mM**).**

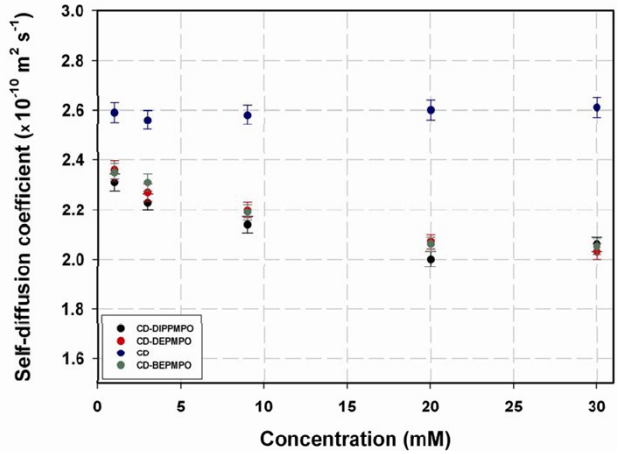


FIG. S5. Evolution of the self-diffusion coefficient D of the three CD-nitrone derivatives as a function of the molar concentration in D_2O at 300 K (the reference compound used was the hydrochloride salt of mono-6-deoxy-6-amino-permethyl-β-cyclodextrin which do not aggregate in this concentration window due to its polar head).

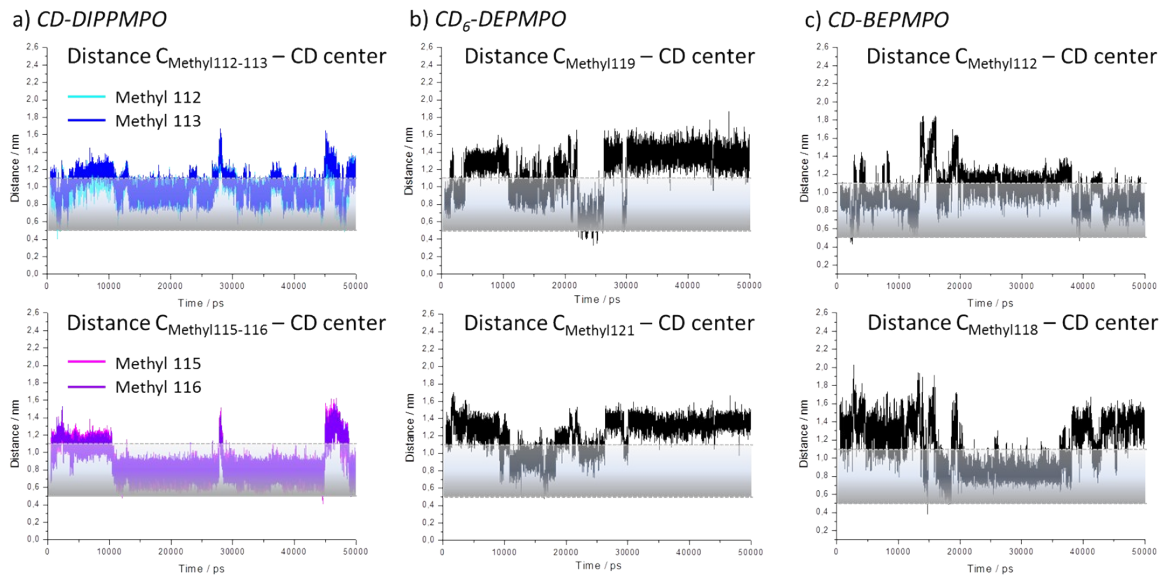


FIG. S6. Time evolution of the distances between guest alkyl groups and the center of permethylated β-CD for (a) CD-DIPPMPO, (b) CD_6-DEPMPO and (c) CD-BEPMPO.

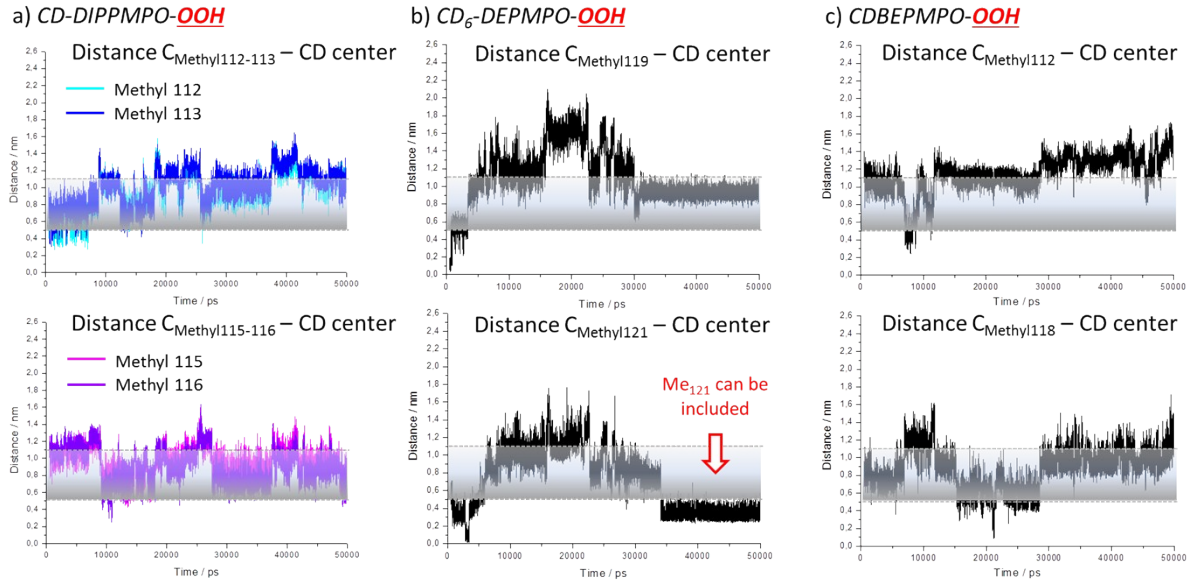


Fig. S7. Time evolution of the distances between guest alkyl groups and the center of permethylated β-CD for (a) CD-DIPPMPO-OOH, (b) CD_6-DEPMPO-OOH and (c) CD-BEPMPO-OOH.

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