SUPPORT INFORMATION:

Diethyl (2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)benzyl) phosphate

Gabriel P. da Costa,1 Diego Alves1 and Márcio S. Silva 1*

¹ G.P. da Costa, Prof. Dr. D. Alves, Prof. Dr. M.S. Silva, Laboratório de Síntese Orgânica Limpa – LASOL, CCQFA, Universidade Federal de Pelotas – UFPel, P. O. Box 354, 96010-900, Pelotas, RS, Brazil

E-mail: silva.ms@ufpel.edu.br (MSS)

Contents

Table S1 - 1H and 13C Chemical shifts of compound 3		S2
Selected spectra of pro	oducts	S3

Table S1. $^1\mathrm{H}$ and $^{13}\mathrm{C}$ Chemical shifts, coupling constants and HMBC 2D correlations of **3**.

Number	¹H (ppm)	¹³ C (ppm)	¹³ C HMBC
1	5.12 (dd, J_{H-P} = 13.1 Hz and J_{H-H} = 5.8 Hz)	65.2 (d, J _{C-P} = 165.0 Hz)	C2, C3, C7
2		133.4	
3	7.99 (d, $J_{H-H} = 8.0 \text{ Hz}$)	129.9 (d, J _{C-P} = 4.1 Hz)	C1, C5, C7
4	7.54 (dd, J_{H-H} = 7.6 and 7.1 Hz)	130.3 (d, J _{C-P} = 2.4 Hz)	C2, C6
5	7.46 – 7.40 (m)	129.3 (d, J _{C-P} = 2.6 Hz)	C3, C7
6	7.37 – 7.33 (m)	123.4	C2, C4, C7
7		135.6 (d, J _{C-P} = 9.1 Hz)	
8	8.43 (s)	123.3	C9
9		147.6	
10		130.1	
11, 11′	7.82 (d, $J_{H-H} = 7.0 \text{ Hz}$)	126.0	C9, C11, C13
12, 12'	7.46 – 7.40 (m)	129.0	C10, C11, C12
13	7.37 – 7.33 (m)	128.5	C11
14	4.16 – 4.00 (m)	63.7 (d, $J_{C-P} = 7.2 \text{ Hz}$)	C15
14′	4.16 – 4.00 (m)	63.4 (d, $J_{C-P} = 7.1 \text{ Hz}$)	C15'
15	1.28 (t, $J_{H-H} = 7.0 \text{ Hz}$)	16.6 (d, $J_{C-P} = 5.5 \text{ Hz}$)	C14
15′	1.21 (t, J _{H-H} = 7.1 Hz)	16.5 (d, $J_{C-P} = 5.6 \text{ Hz}$)	C14'
ОН	5.02 (dd, J_{H-P} = 16.5 and J_{H-H} = 5.8 Hz)		C1

Selected spectra of products

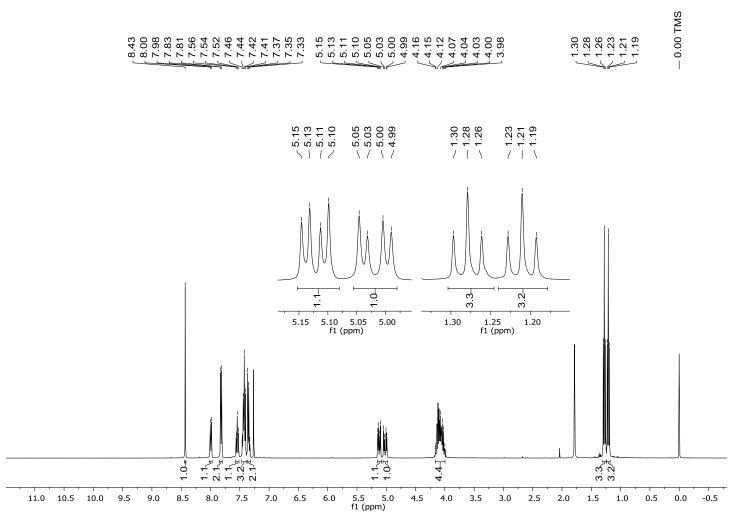


Figure S1:1H NMR (400 MHz, CDCl₃) spectrum of compound 3.

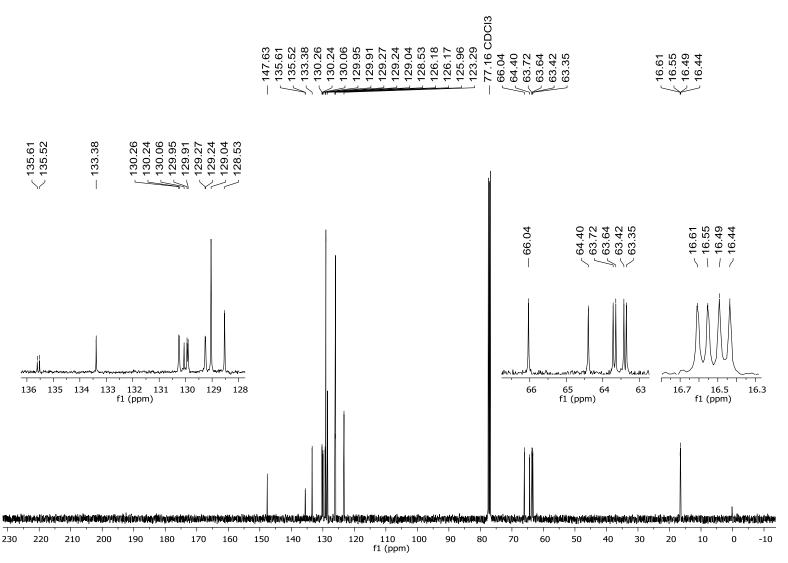


Figure S2:13C{1H} NMR (100 MHz, CDCl₃) spectrum of compound 3.

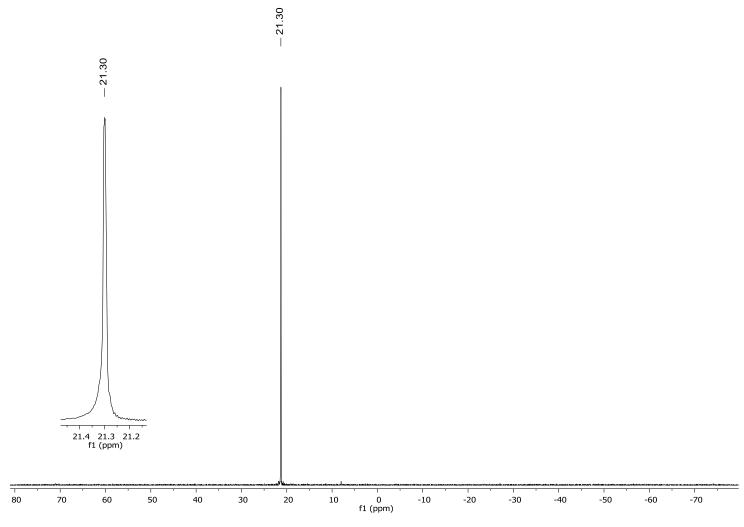


Figure S3: ³¹P NMR (162 MHz, CDCl₃) spectrum of compound 3.

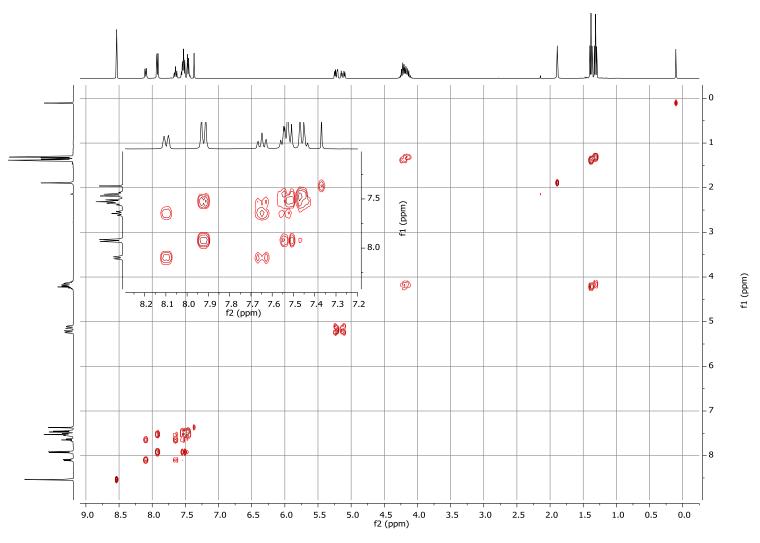


Figure S4: COSY correlations of compound 3 in $CDCl_3$.

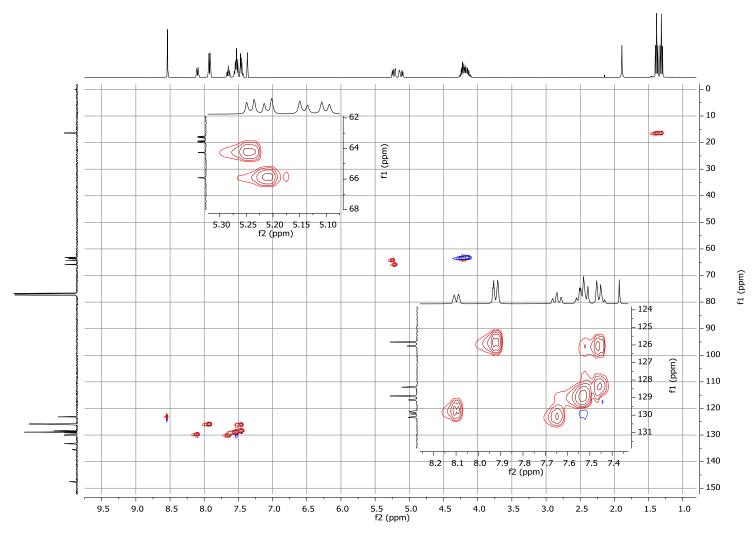


Figure S5: HSQC correlations of compound 3 in CDCl₃.

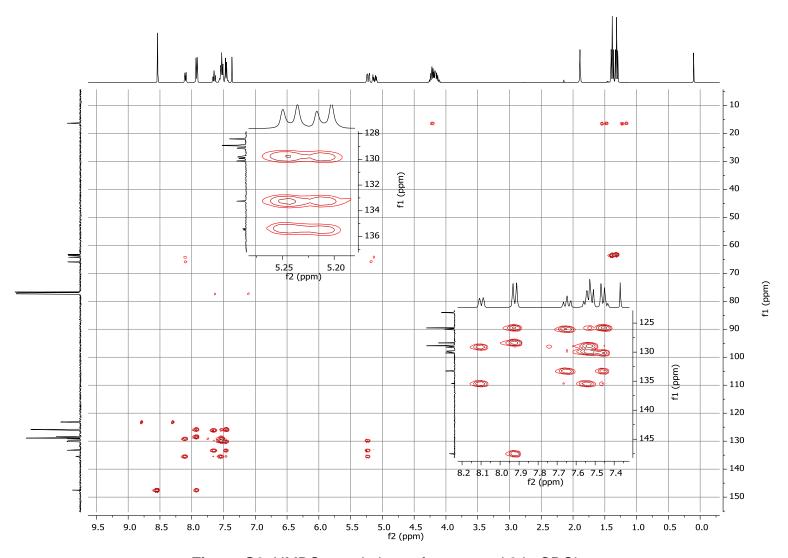


Figure S6: HMBC correlations of compound 3 in CDCl₃.

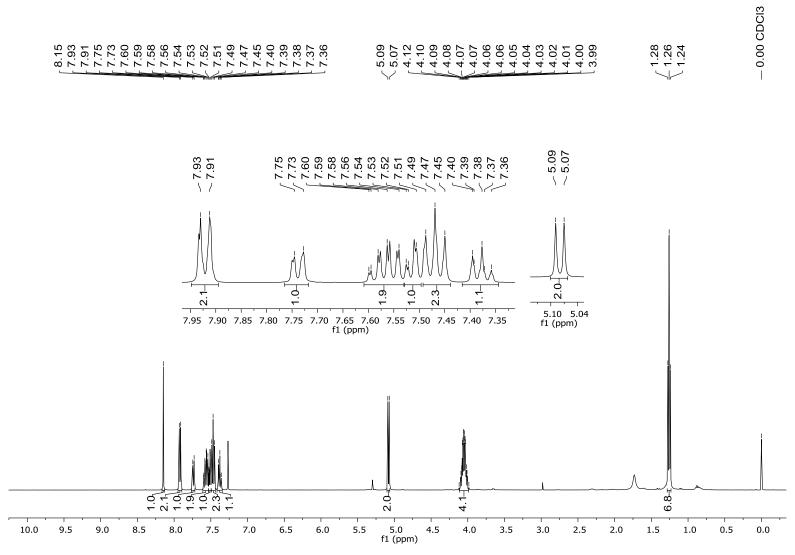


Figure S7: ¹H NMR (400 MHz, CDCl₃) spectrum of compound 4.

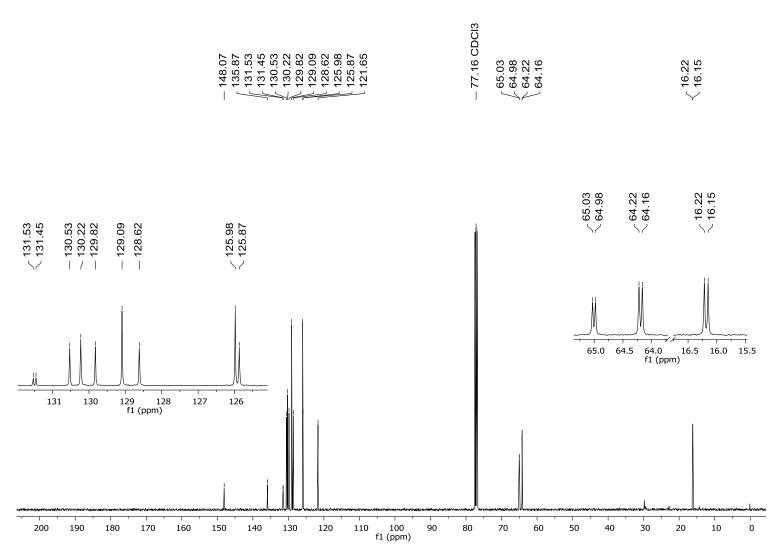


Figure S8: $^{13}C\{^{1}H\}$ NMR (100 MHz, CDCl₃) spectrum of compound 4.

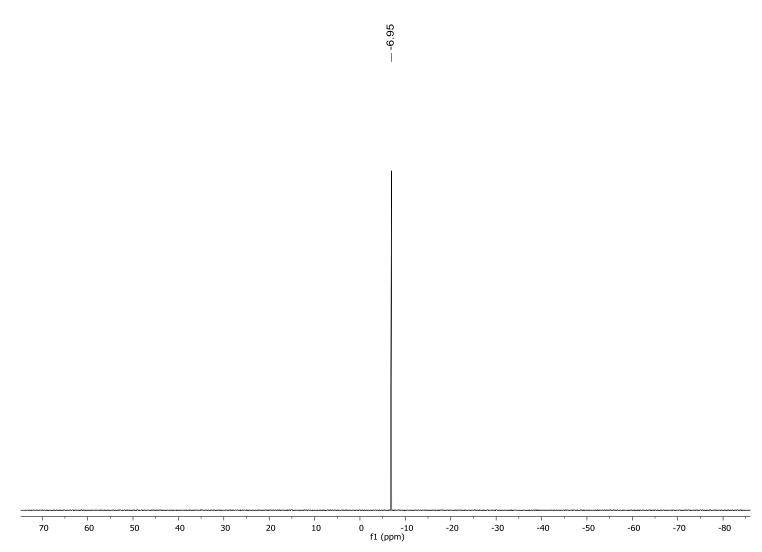


Figure S9: ³¹P NMR (162 MHz, CDCl₃) spectrum of compound 4.

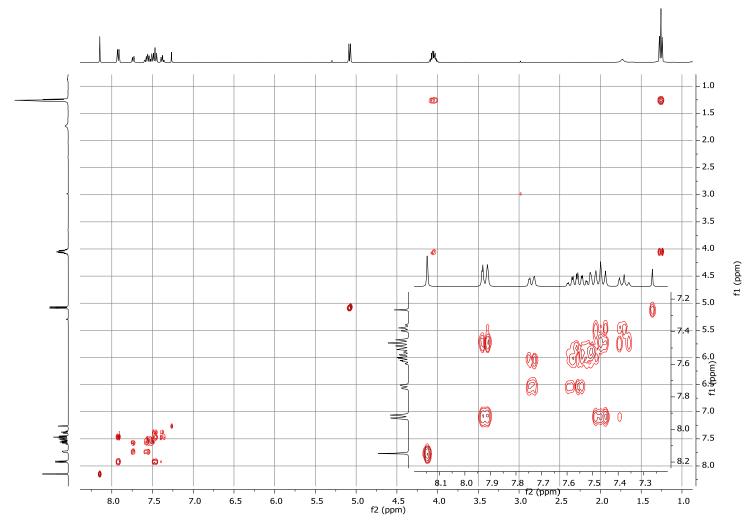


Figure \$10: COSY correlations of compound 4 in CDCl₃.

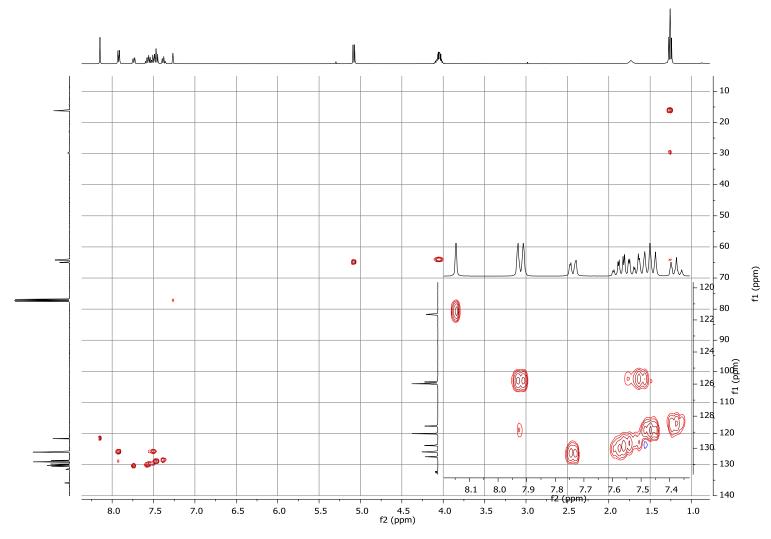


Figure S11: HSQC correlations of compound 4 in CDCl₃.

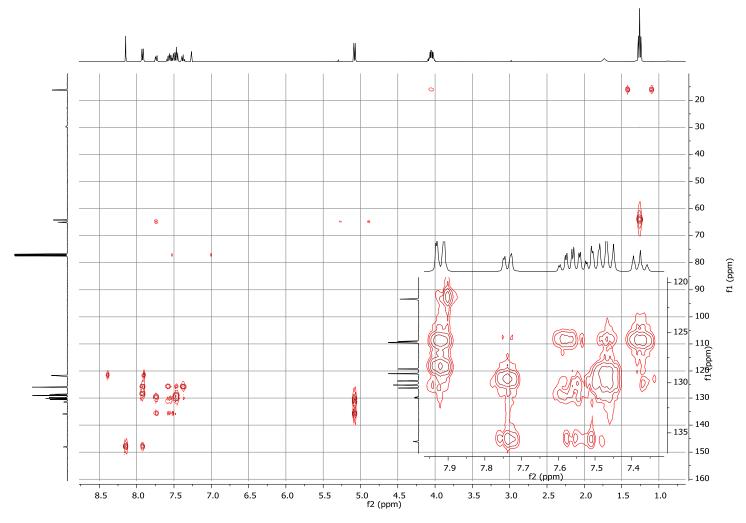


Figure S12: HMBC correlations of compound 4 in CDCl₃.

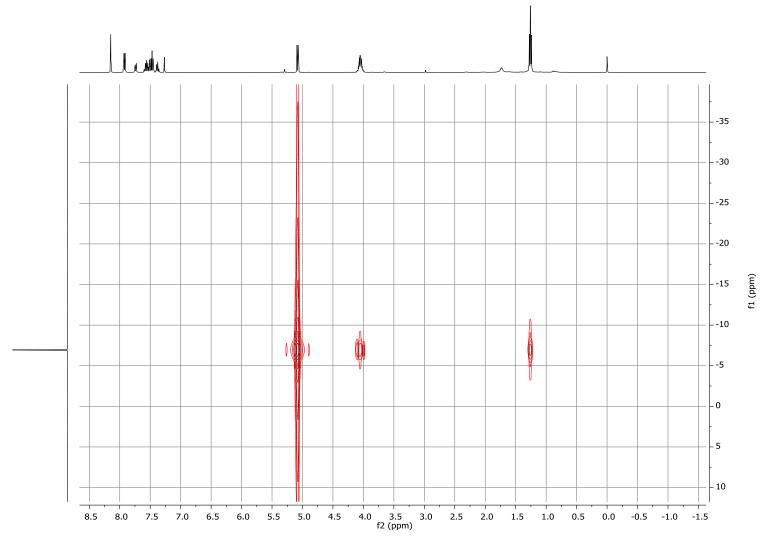


Figure S13: HMBC (¹H-³¹P) correlations of compound 4 in CDCl₃.