

Supporting Information

Octahydroquinoxalin-2(1*H*)-One-Based Aminophosphonic Acids and Their Derivatives – Biological Activity Towards Cancer Cells

Jakub Iwanejko ¹, Elżbieta Wojaczyńska ^{1,*}, Eliza Turlej ², Magdalena Maciejewska ² and Joanna Wietrzyk ²

¹ Faculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland; jakub.iwanejko@pwr.edu.pl

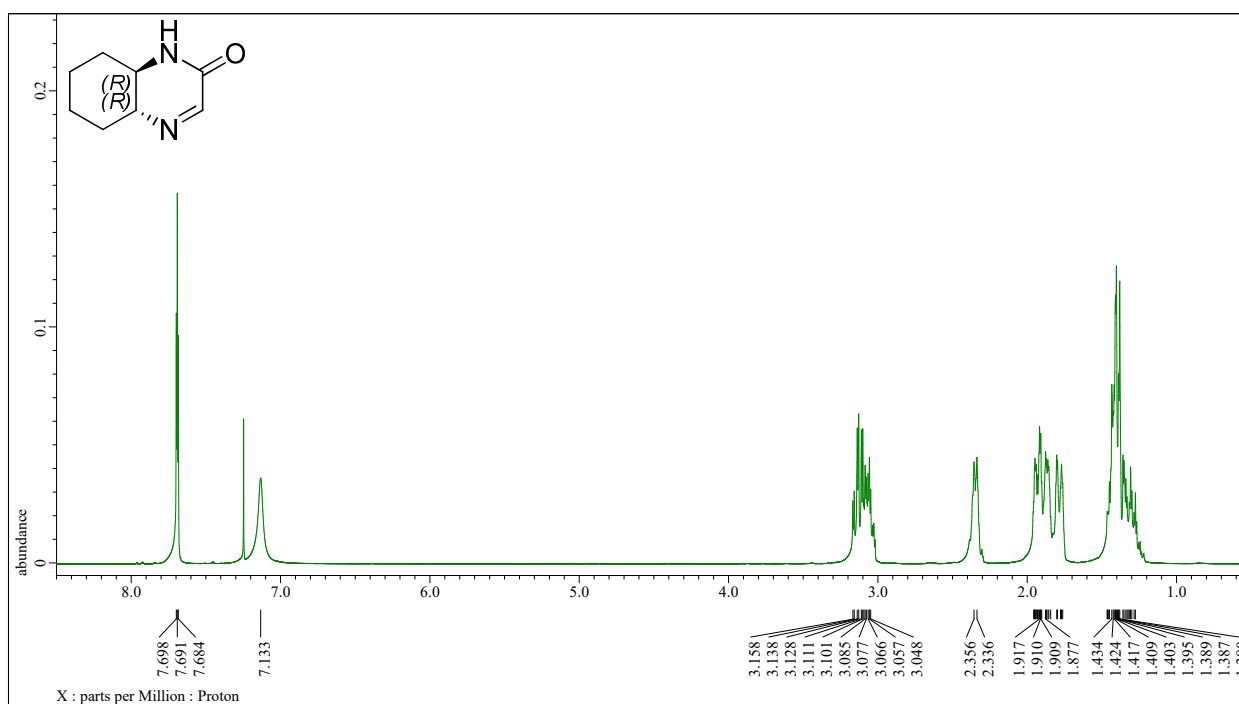
² Department of Experimental Oncology, Hirszfeld Institute of Immunology and Experimental Therapy, Polish Academy of Sciences, Rudolfa Weigla 12, 53-114 Wrocław, Poland; eliza.turlej@hirszfeld.pl (E.T.); magdalena.maciejewska@hirszfeld.pl (M.M.); joanna.wietrzyk@hirszfeld.pl (J.W.)

* Correspondence: elzbieta.wojaczynska@pwr.edu.pl; Tel.: +48-71-3202410

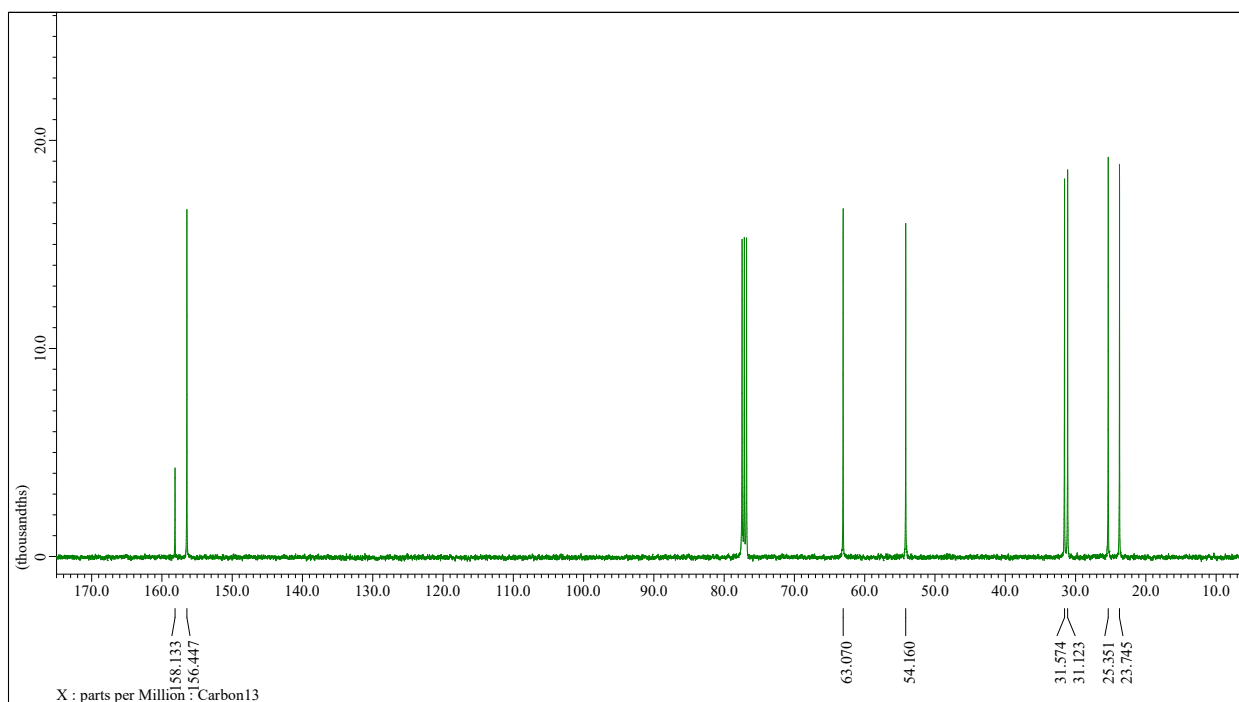
Contents

1. NMR Spectra.....	2
Figure S1. (a) ¹ H NMR and (b) ¹³ C NMR spectra of (1 <i>R</i> ,6 <i>R</i>)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-ene 1.....	2
Figure S2. (a) ¹ H NMR, (b) ¹³ C NMR and (c) ³¹ P NMR spectra of dimethyl-[(1 <i>R</i> ,6 <i>R</i>)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]phosphonate 2a.....	4
Figure S3. (a) ¹ H NMR, (b) ¹³ C NMR and (c) ³¹ P NMR spectra of diphenyl-[(1 <i>R</i> ,6 <i>R</i>)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]phosphonate 2b.....	5
Figure S4. (a) ¹ H NMR, (b) ¹³ C NMR and (c) ³¹ P NMR spectra of dibenzyl-[(1 <i>R</i> ,6 <i>R</i>)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]phosphonate 2c.....	7
Figure S5. (a) ¹ H NMR, (b) ¹³ C NMR and (c) ³¹ P NMR spectra of ethyl-[(1 <i>R</i> ,6 <i>R</i>)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl](phenyl)phosphinate 2d.....	8
Figure S6. (a) ¹ H NMR, (b) ¹³ C NMR and (c) ³¹ P NMR spectra of (1 <i>R</i> ,6 <i>R</i>)-3-oxo-4-(diphenylphosphoryl)-2,5-diazabicyclo[4.4.0]decan 2e.....	10
Figure S7. (a) ¹ H NMR, (b) ¹³ C NMR and (c) ³¹ P NMR spectra of 4-((3 <i>aR</i> ,8 <i>aR</i>)-2,2-dimethyl-6-oxido-4,4,8,8-tetraphenyltetrahydro-[1,3]dioxolo[4,5- <i>e</i>][1,3,2]dioxaphosphepin-6-yl)-(1 <i>R</i> ,6 <i>R</i>)-3-oxo-2,5-diazabicyclo[4.4.0]decan 2f.....	11
Figure S8. (a) ¹ H NMR, (b) ¹³ C NMR and (c) ³¹ P NMR spectra of 4-((3 <i>aR</i> ,8 <i>aR</i>)-2,2-dimethyl-6-oxido-4,4,8,8-tetraphenyltetrahydro-[1,3]dioxolo[4,5- <i>e</i>][1,3,2]dioxaphosphepin-6-yl)-(1 <i>R</i> ,6 <i>R</i>)-3-oxo-2,5-diazabicyclo[4.4.0]decan 2g.....	13
Figure S9. (a) ¹ H NMR, (b) ¹³ C NMR and (c) ³¹ P NMR spectra of [(1 <i>R</i> ,6 <i>R</i>)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid 3a.....	14
Figure S10. (a) ¹ H NMR, (b) ¹³ C NMR and (c) ³¹ P NMR spectra of [4-phenyl-(1 <i>R</i> ,6 <i>R</i>)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid 3b.....	16

1. NMR Spectra

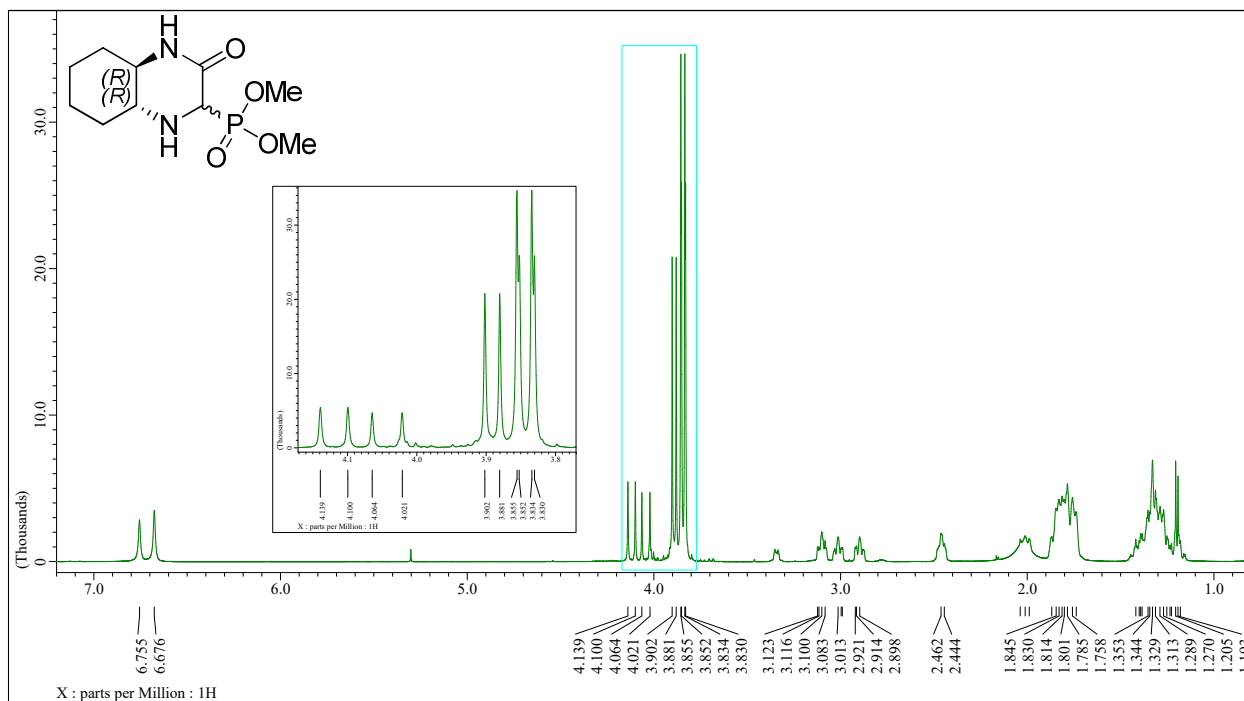


(a)

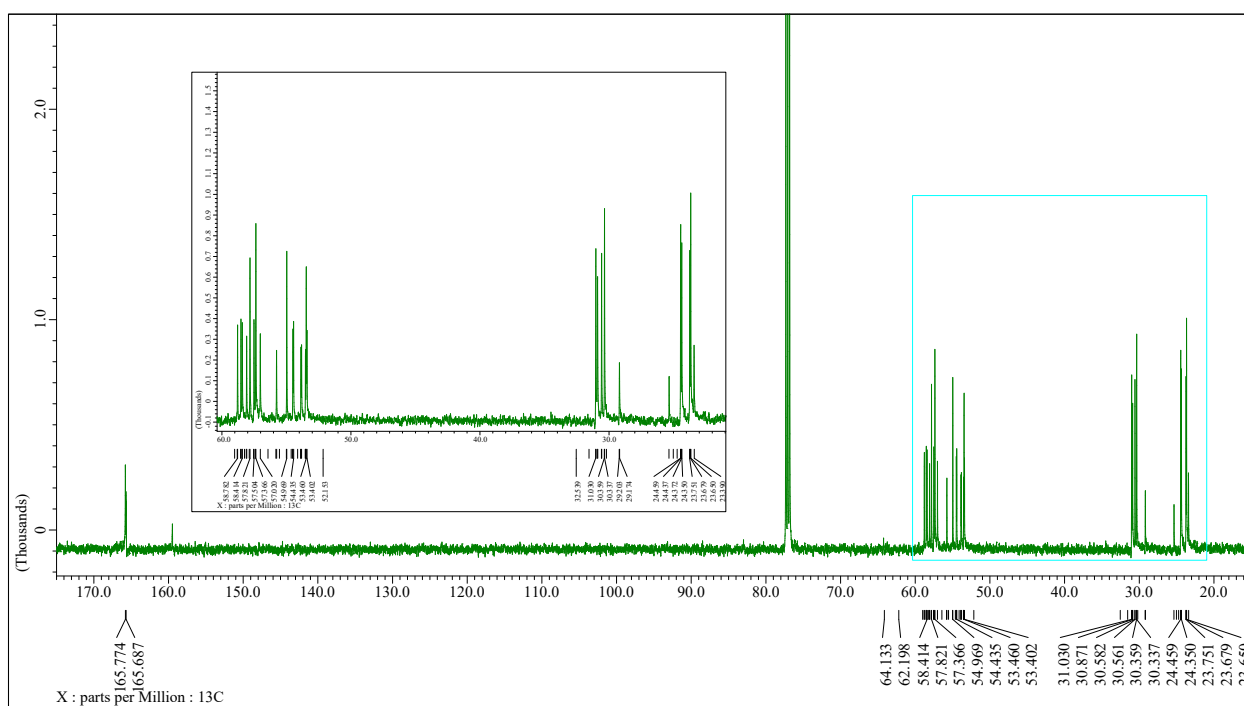


(b)

Figure S1. (a) ^1H NMR and (b) ^{13}C NMR spectra of (1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-ene 1.



(a)



(b)

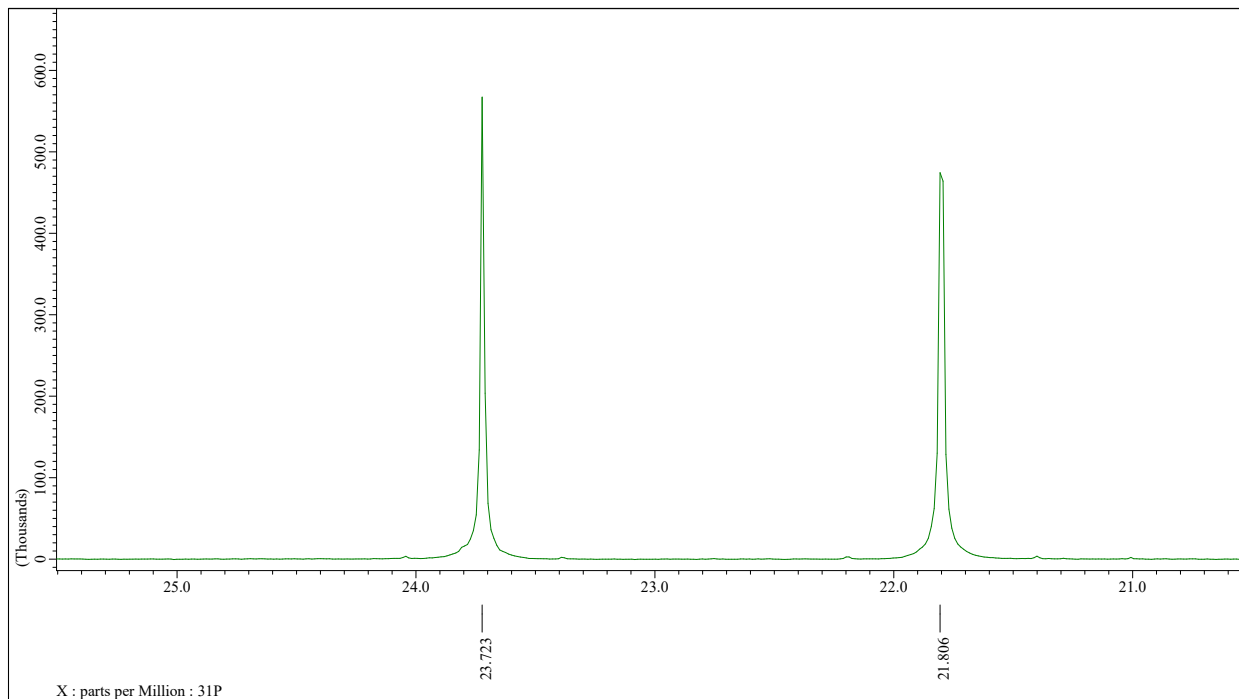
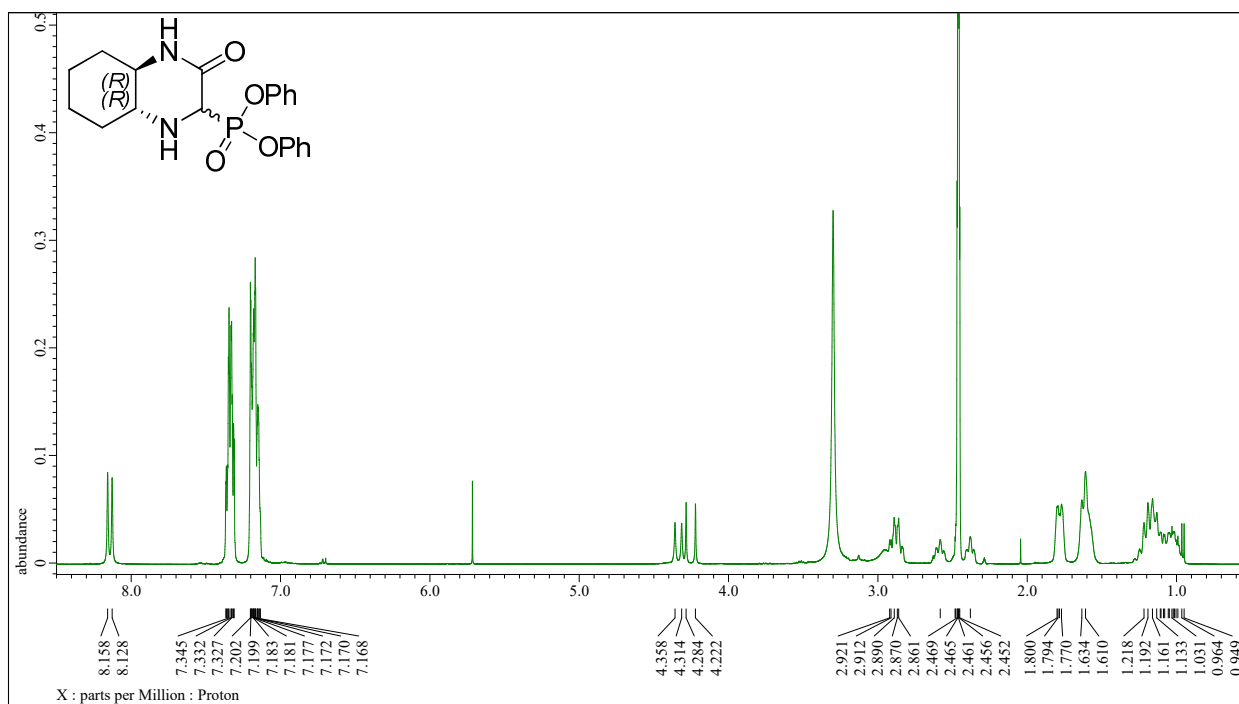


Figure S2. (a) ^1H NMR, (b) ^{13}C NMR and (c) ^{31}P NMR spectra of dimethyl-[(1R,6R)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]phosphonate 2a.



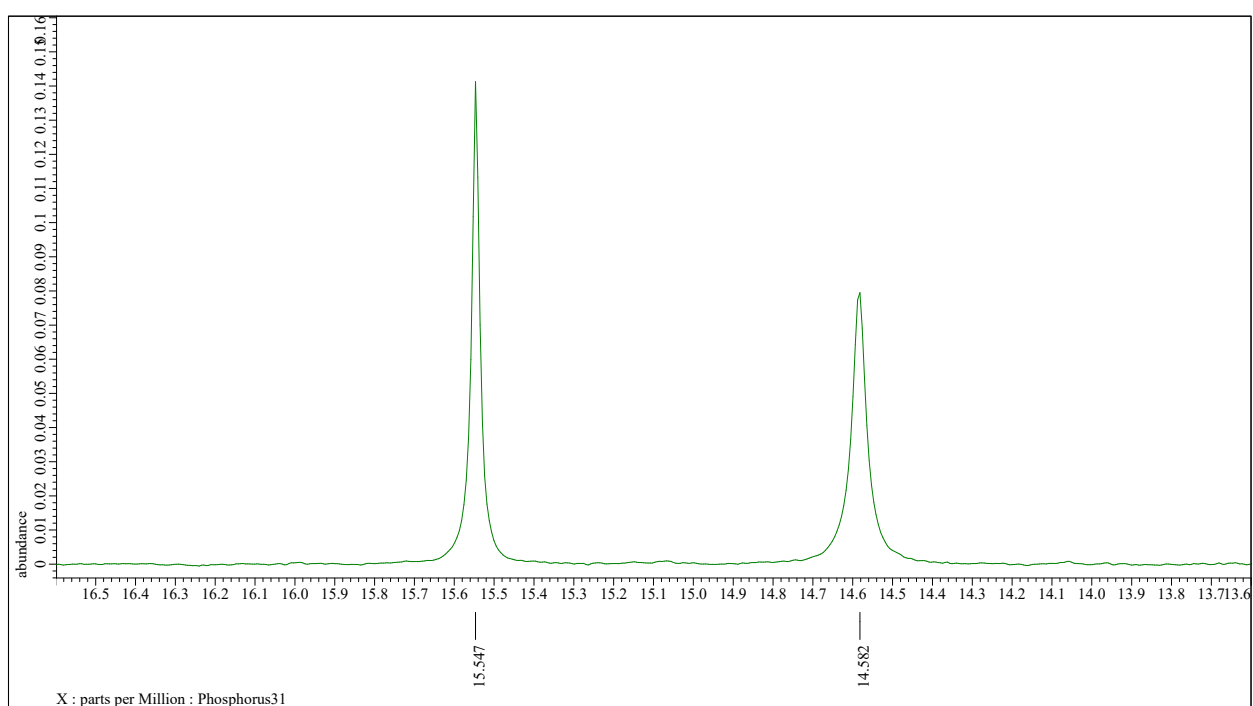
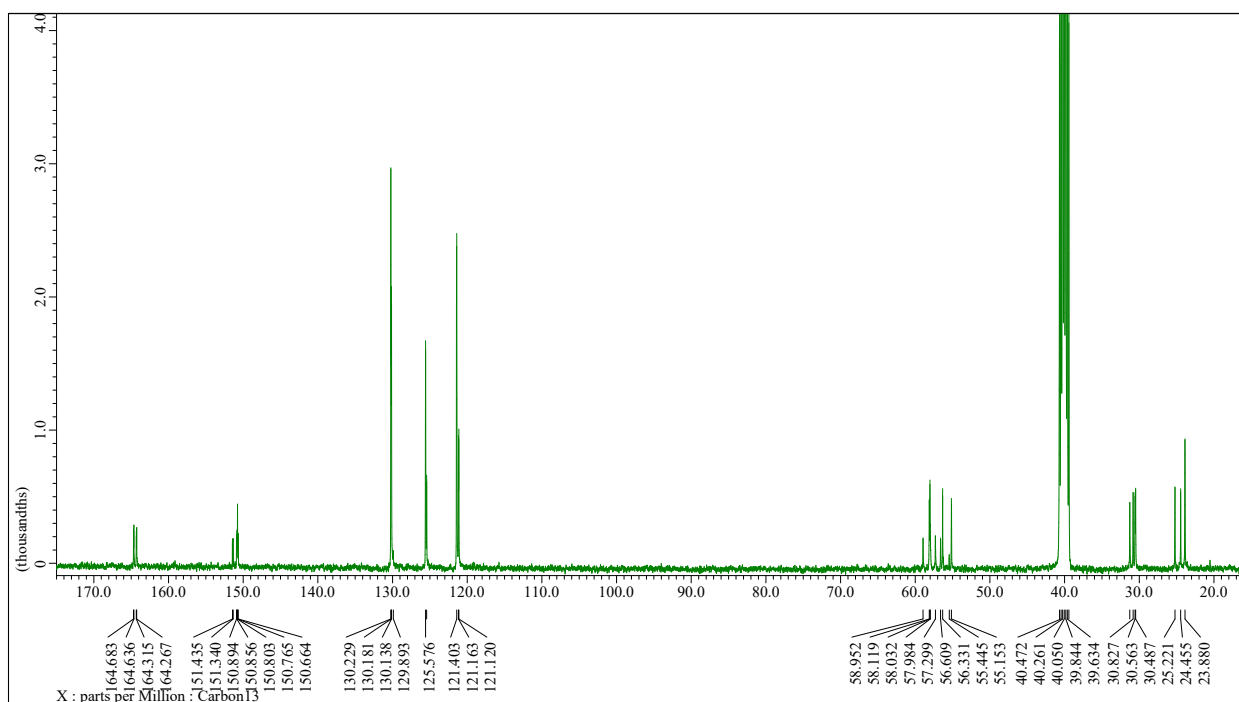
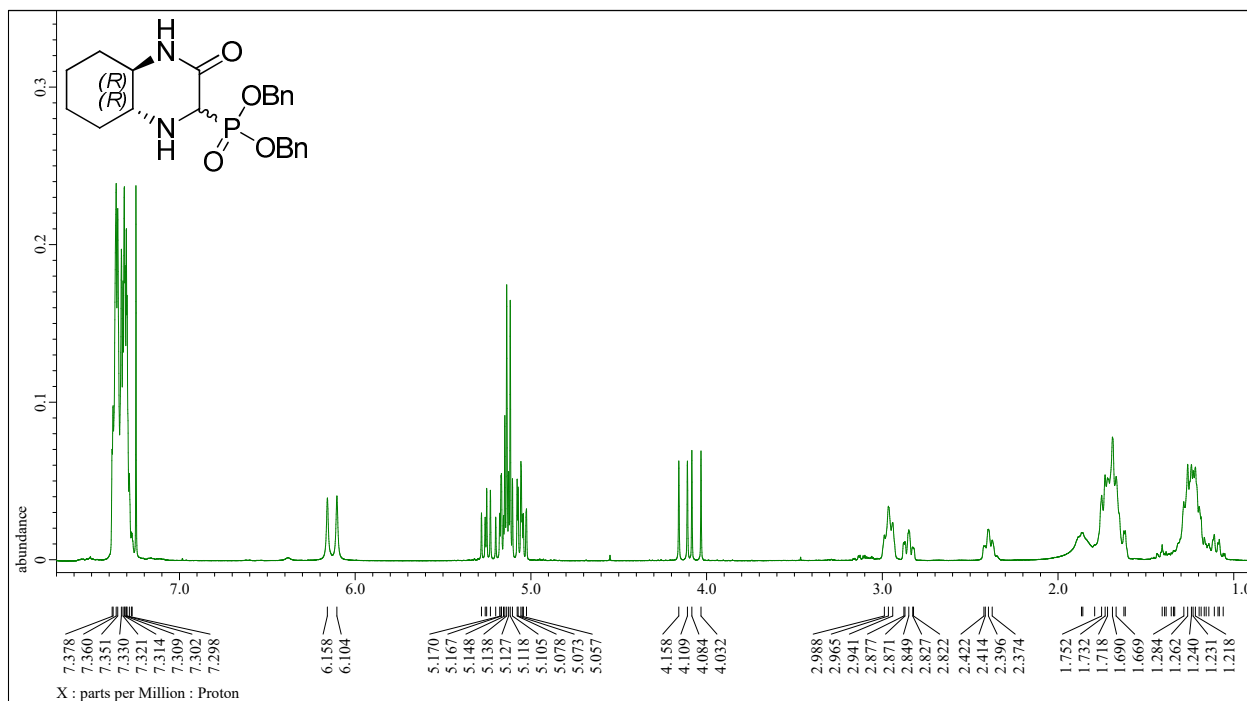
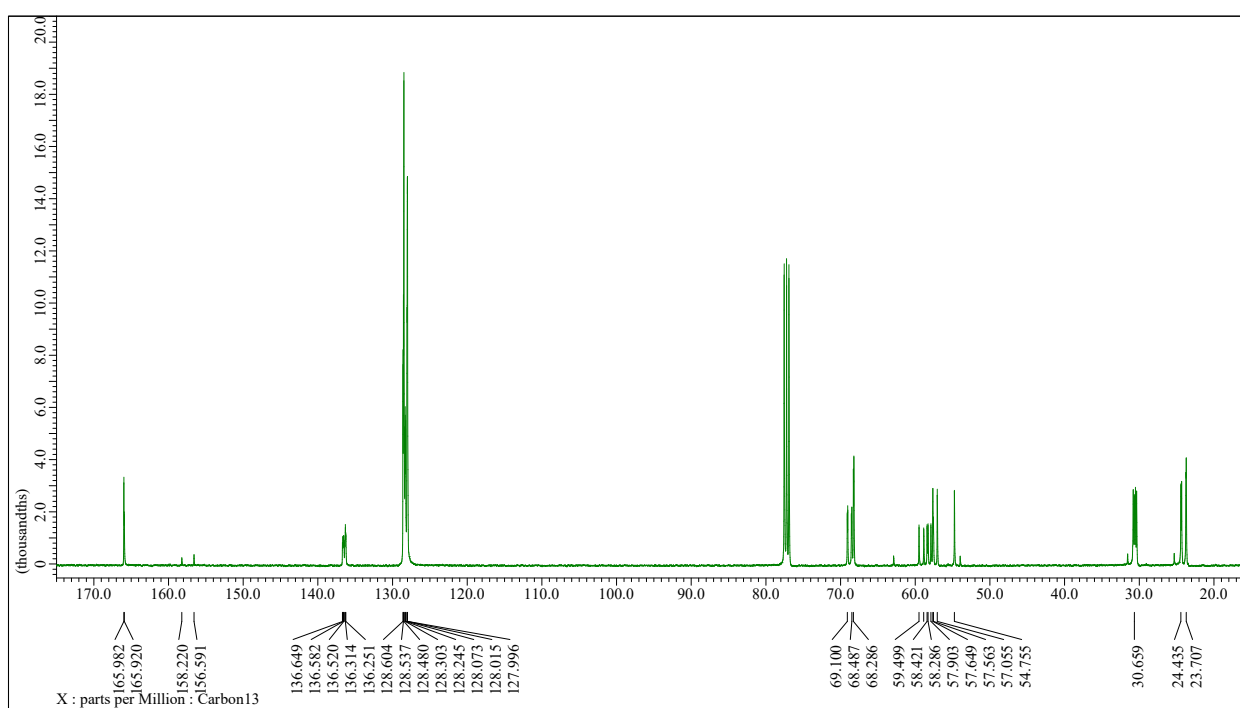


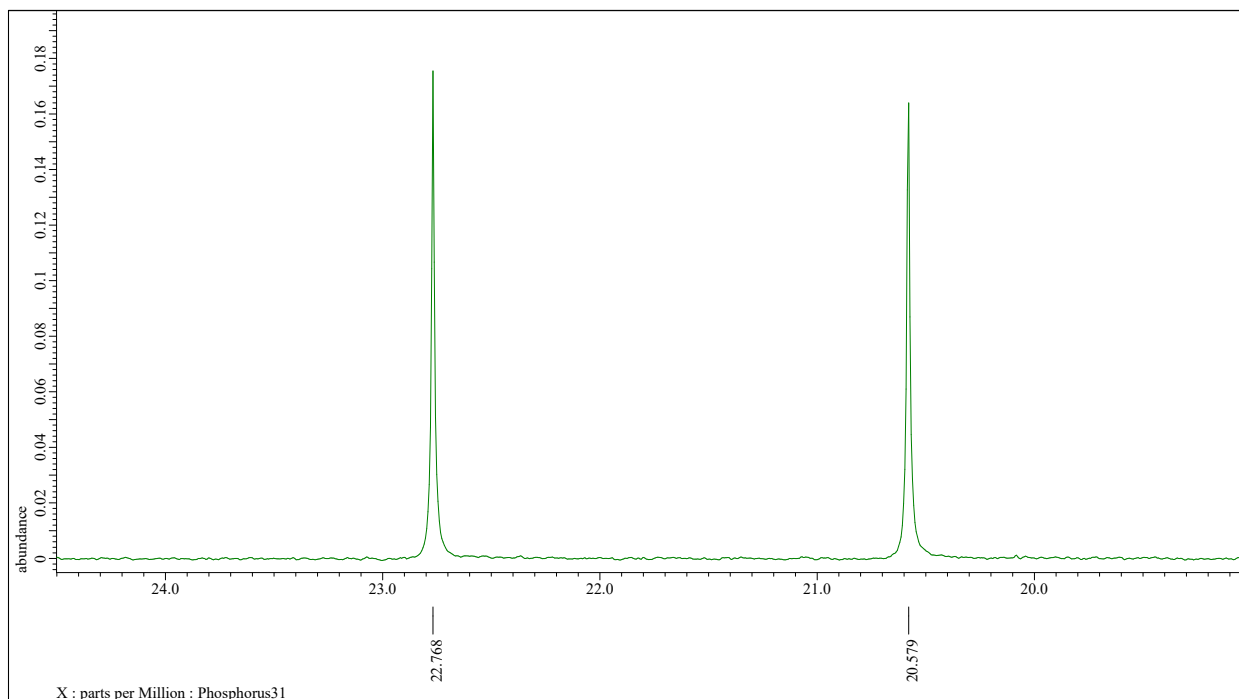
Figure S3. (a) ^1H NMR, (b) ^{13}C NMR and (c) ^{31}P NMR spectra of diphenyl-[(1R,6R)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]phosphonate 2b.



(a)

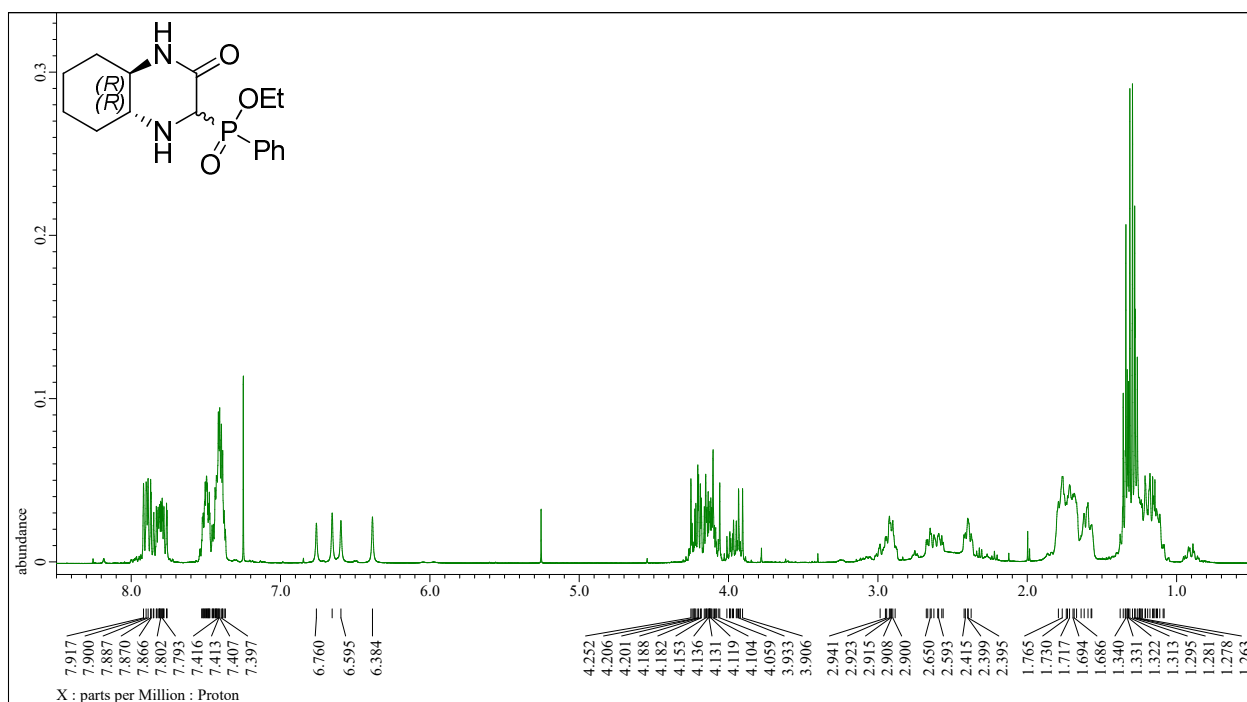


(b)

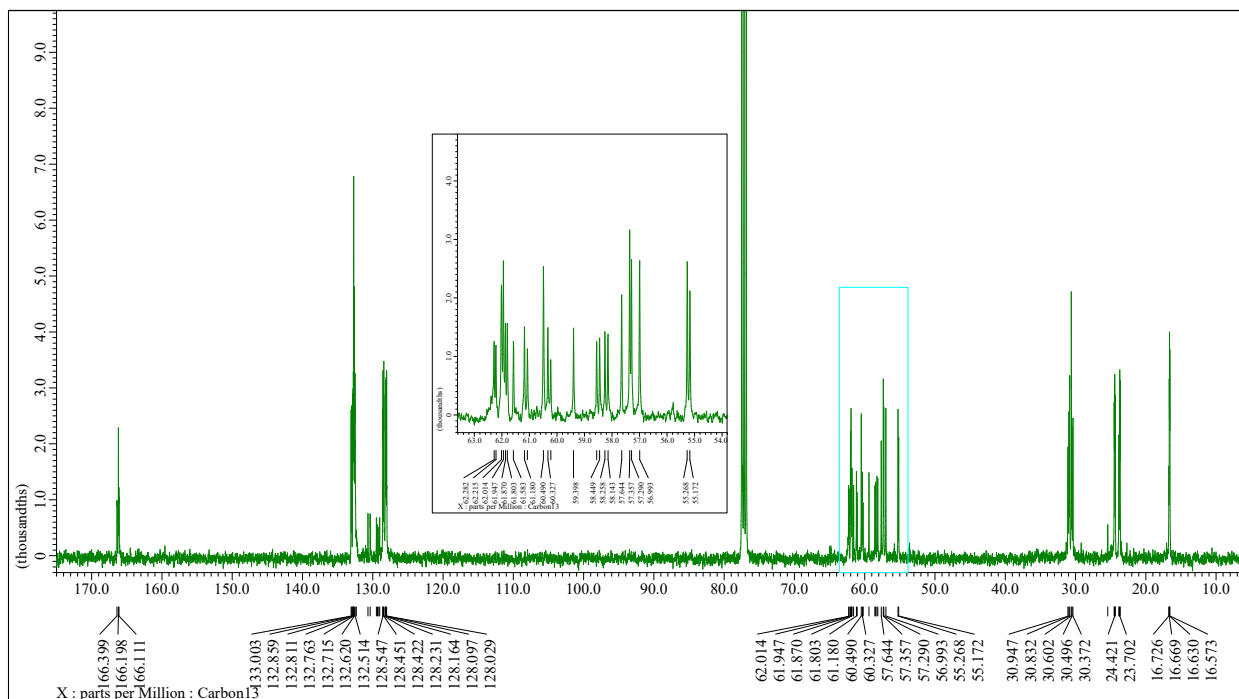


(c)

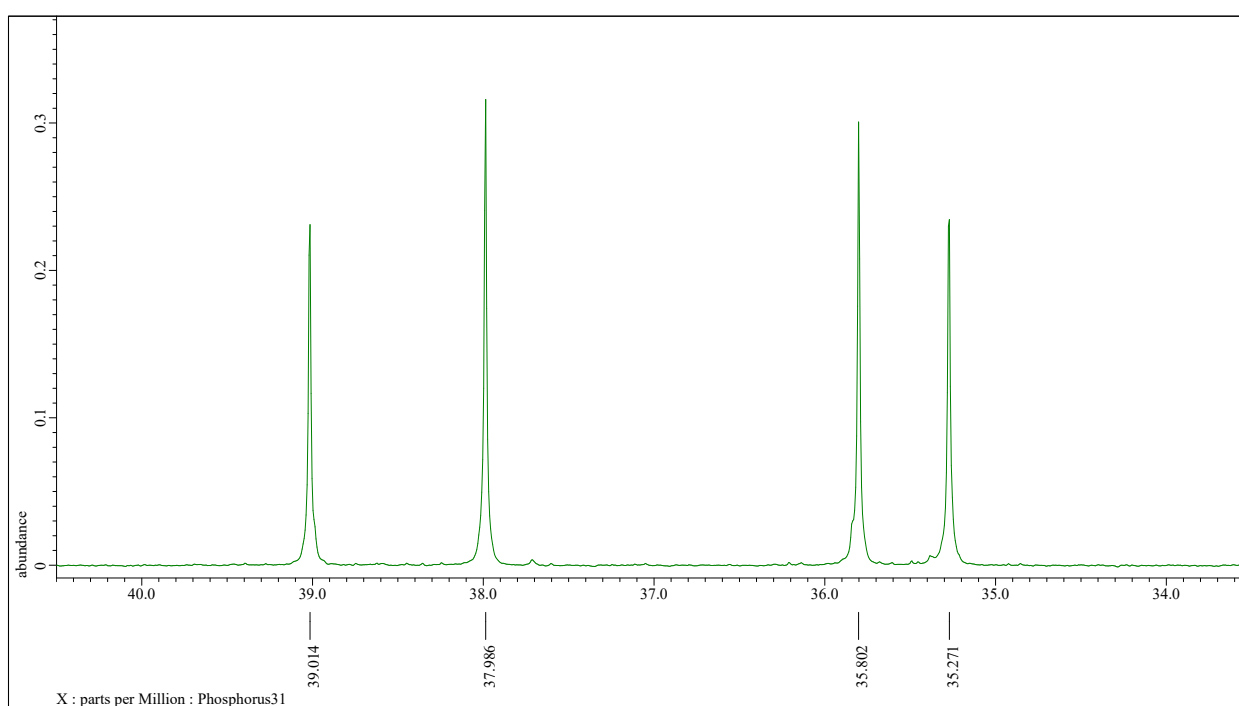
Figure S4. (a) ^1H NMR, (b) ^{13}C NMR and (c) ^{31}P NMR spectra of dibenzyl-[(1R,6R)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]phosphonate 2c.



(a)

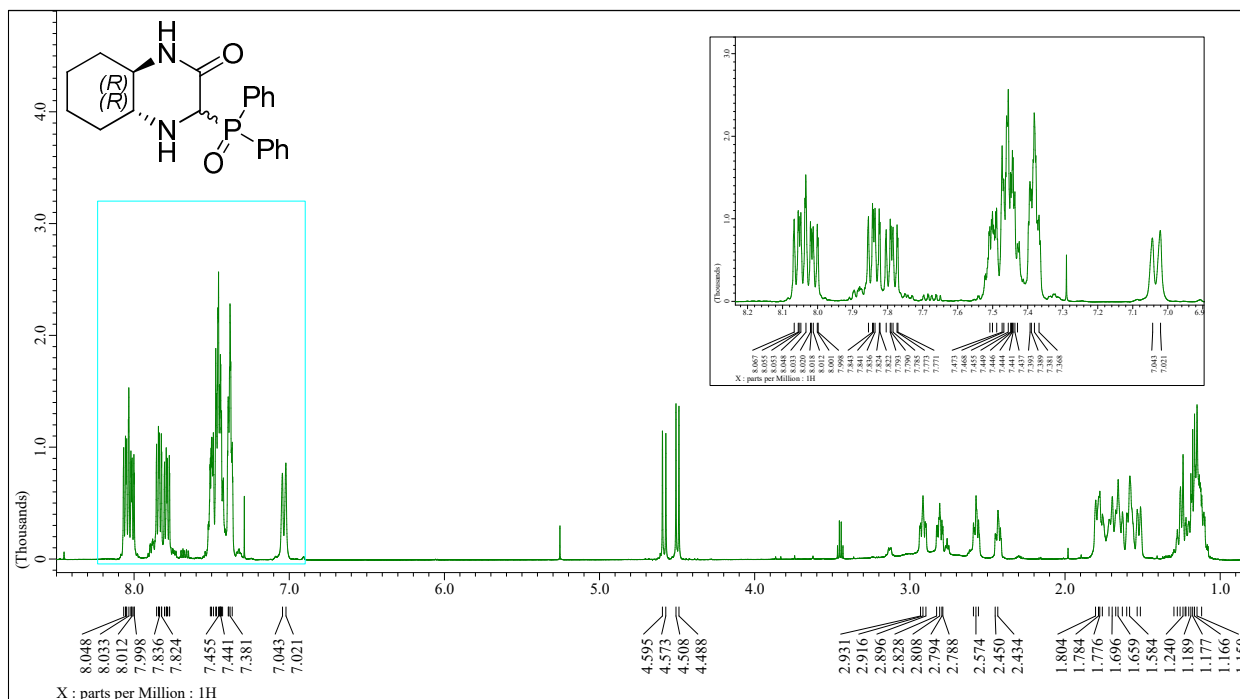


(b)

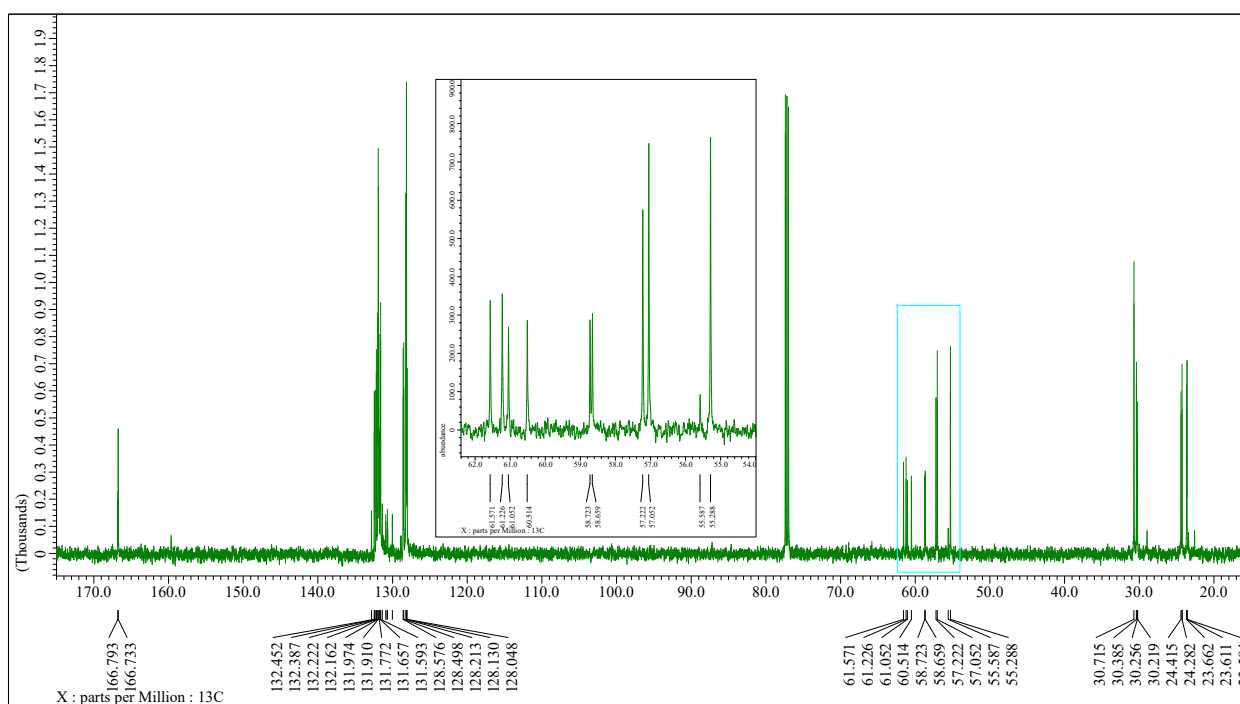


(c)

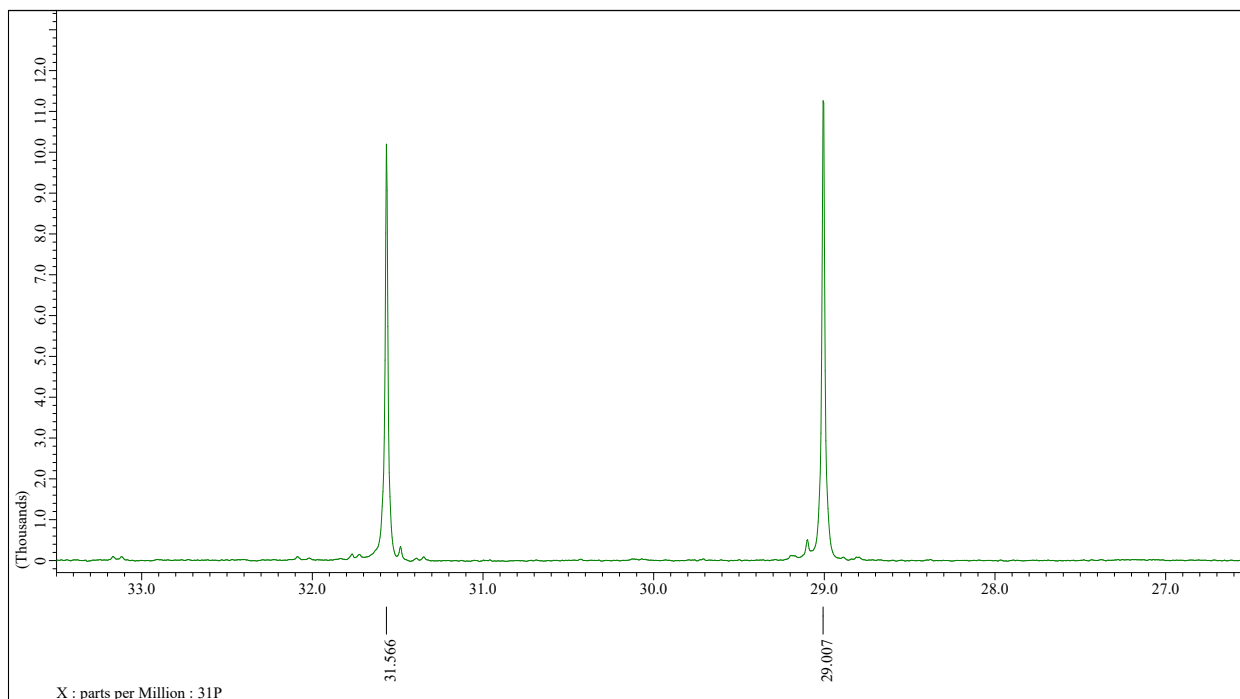
Figure S5. (a) ^1H NMR, (b) ^{13}C NMR and (c) ^{31}P NMR spectra of ethyl-[(1R,6R)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl](phenyl)phosphinate 2d.



(a)

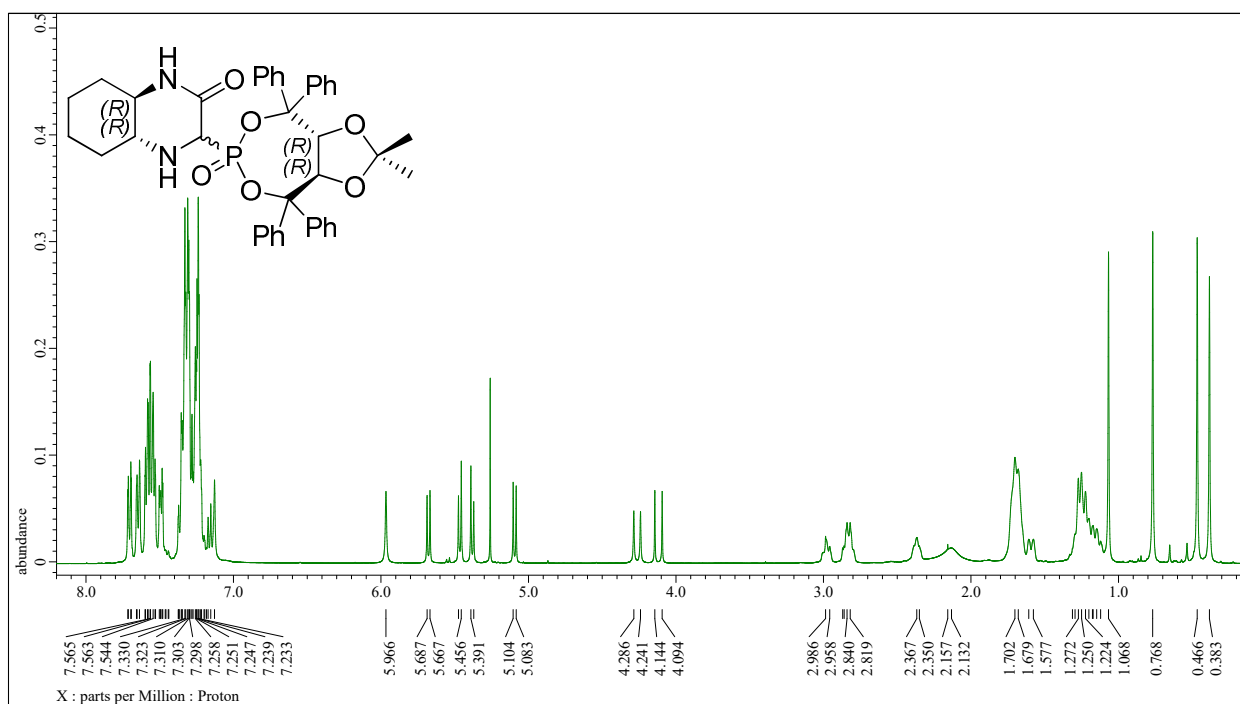


(b)



(c)

Figure S6. (a) ^1H NMR, (b) ^{13}C NMR and (c) ^{31}P NMR spectra of (1*R*,6*R*)-3-oxo-4-(diphenylphosphoryl)-2,5-diazabicyclo[4.4.0]decan 2e.



(a)

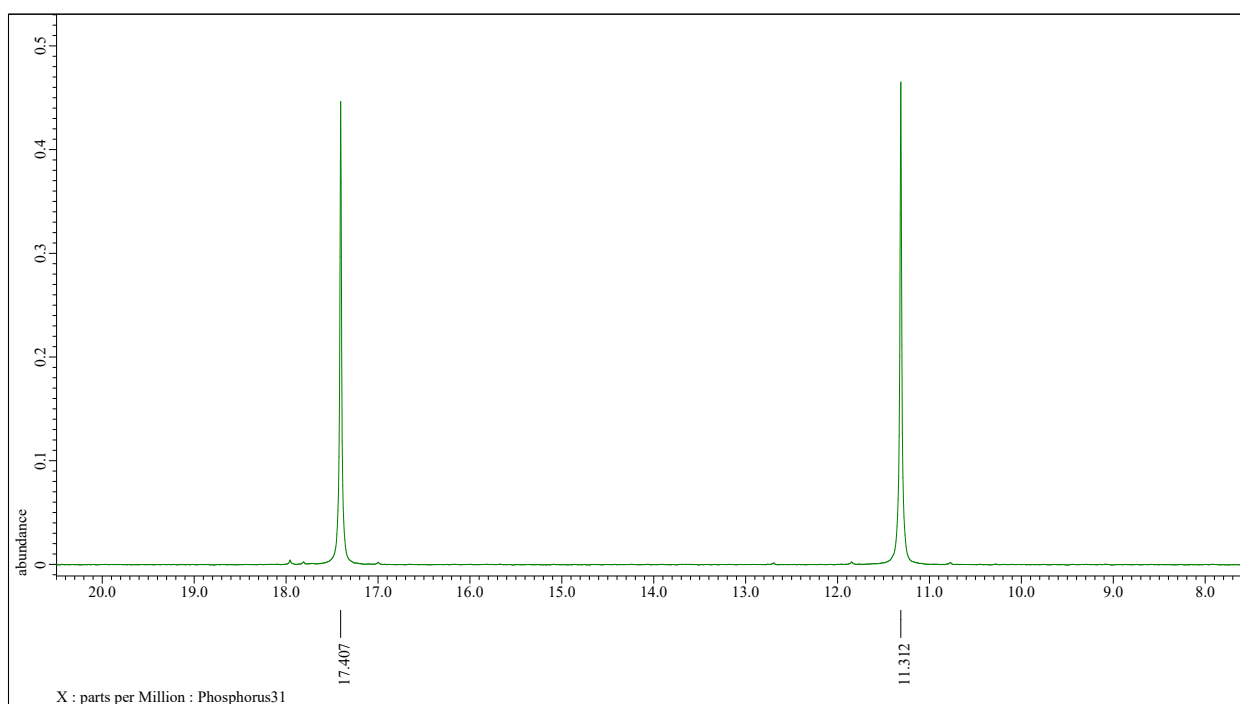
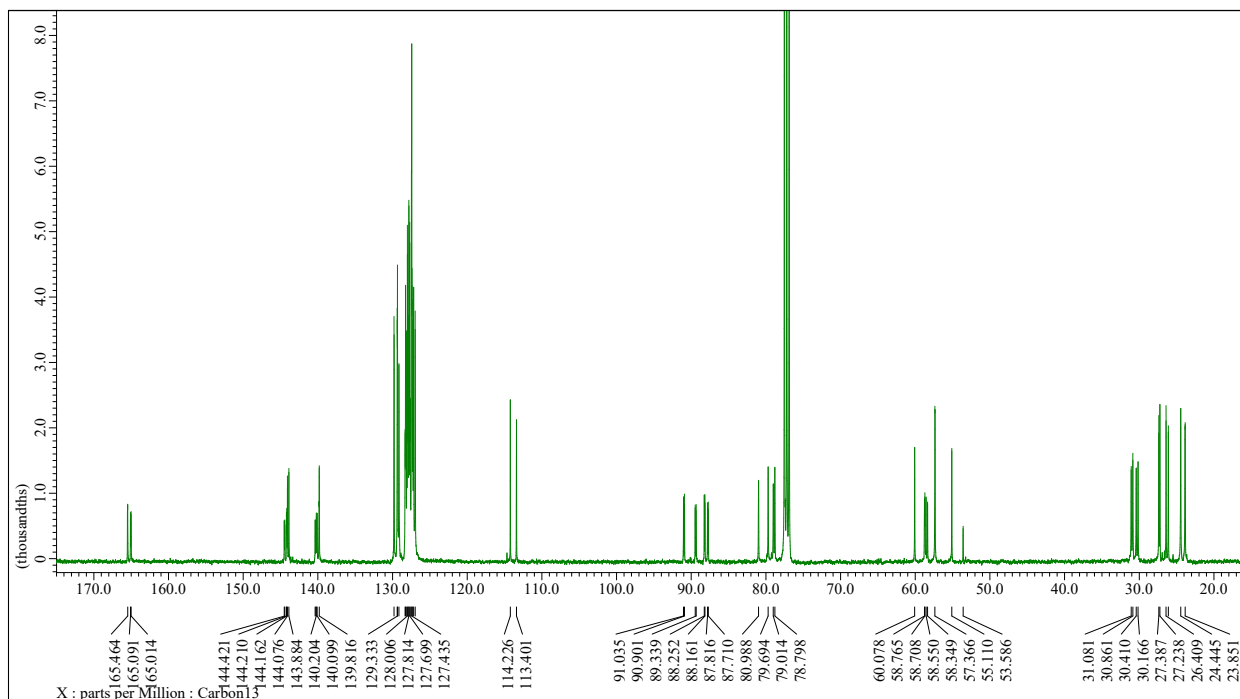
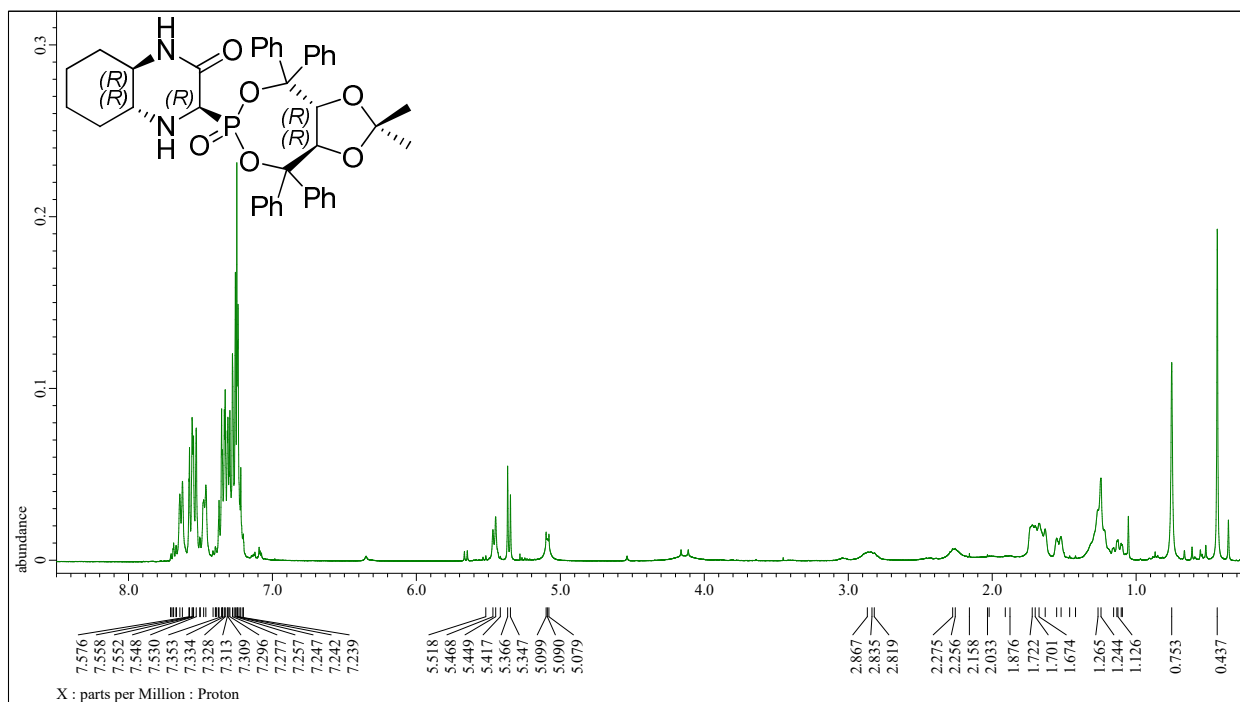
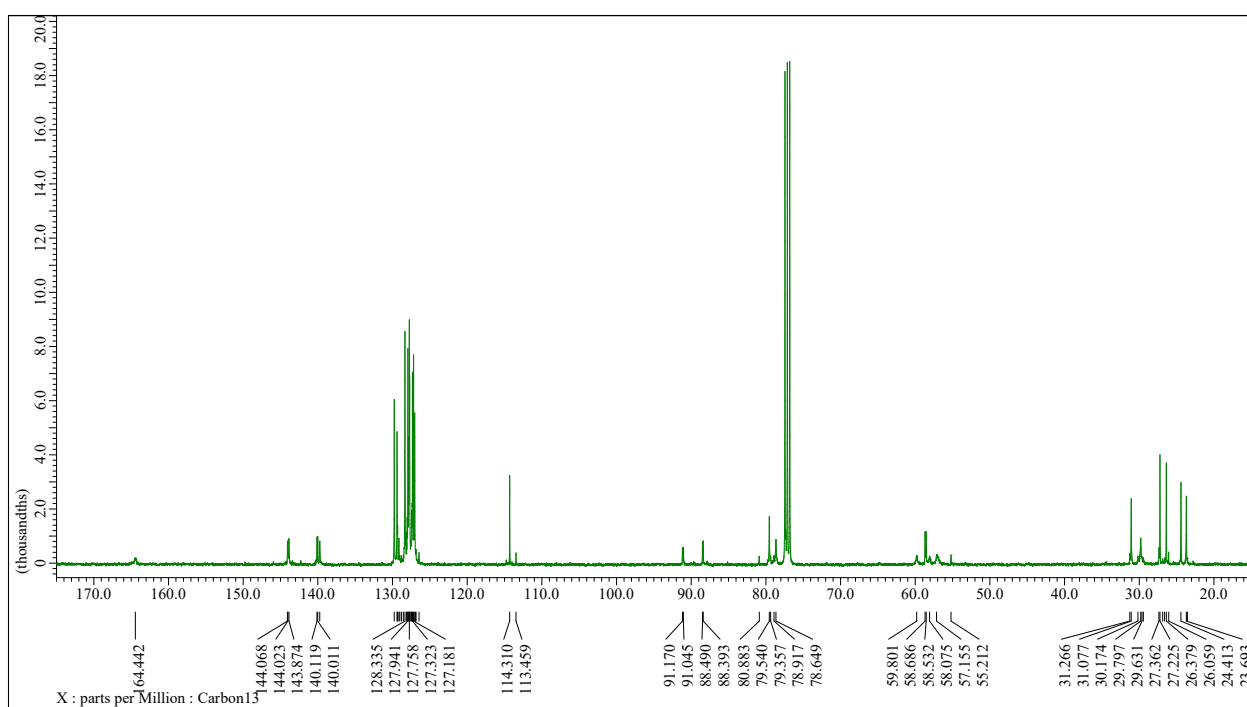


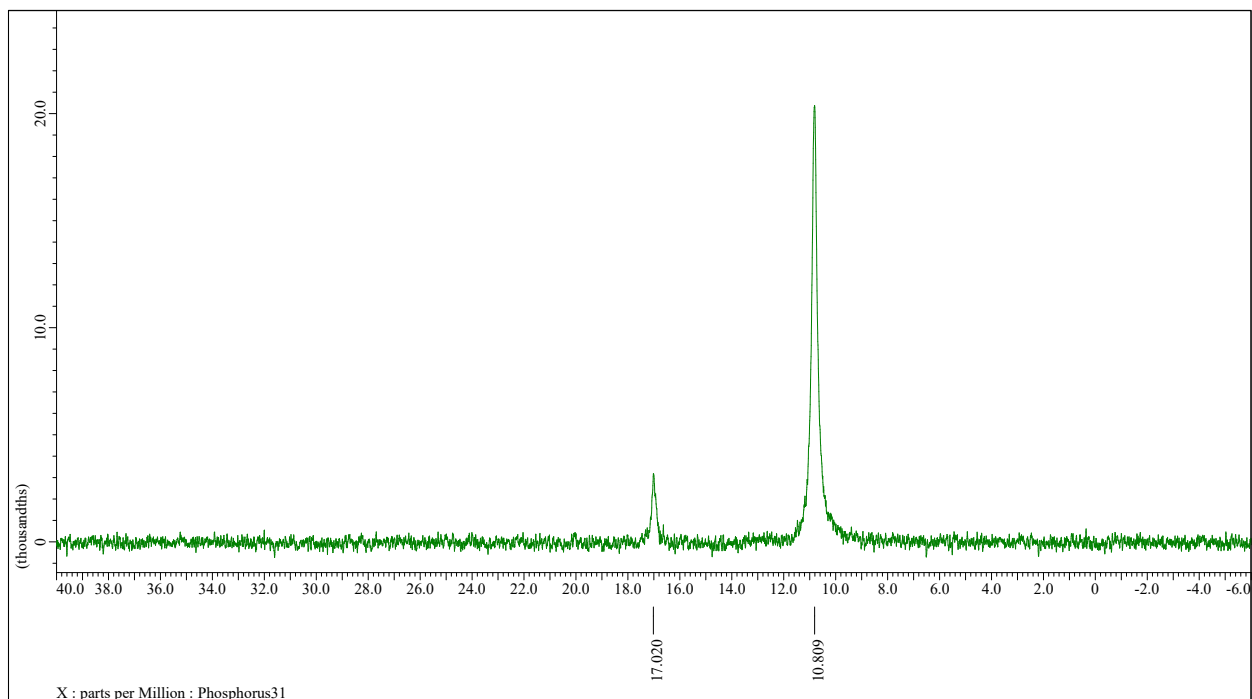
Figure 7. (a) ^1H NMR, (b) ^{13}C NMR and (c) ^{31}P NMR spectra of 4-((3*aR*,8*aR*)-2,2-dimethyl-6-oxido-4,4,8,8-tetraphenyltetrahydro-[1,3]dioxolo[4,5-*e*][1,3,2]dioxaphosphepin-6-yl)-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]decan 2*f*.



(a)

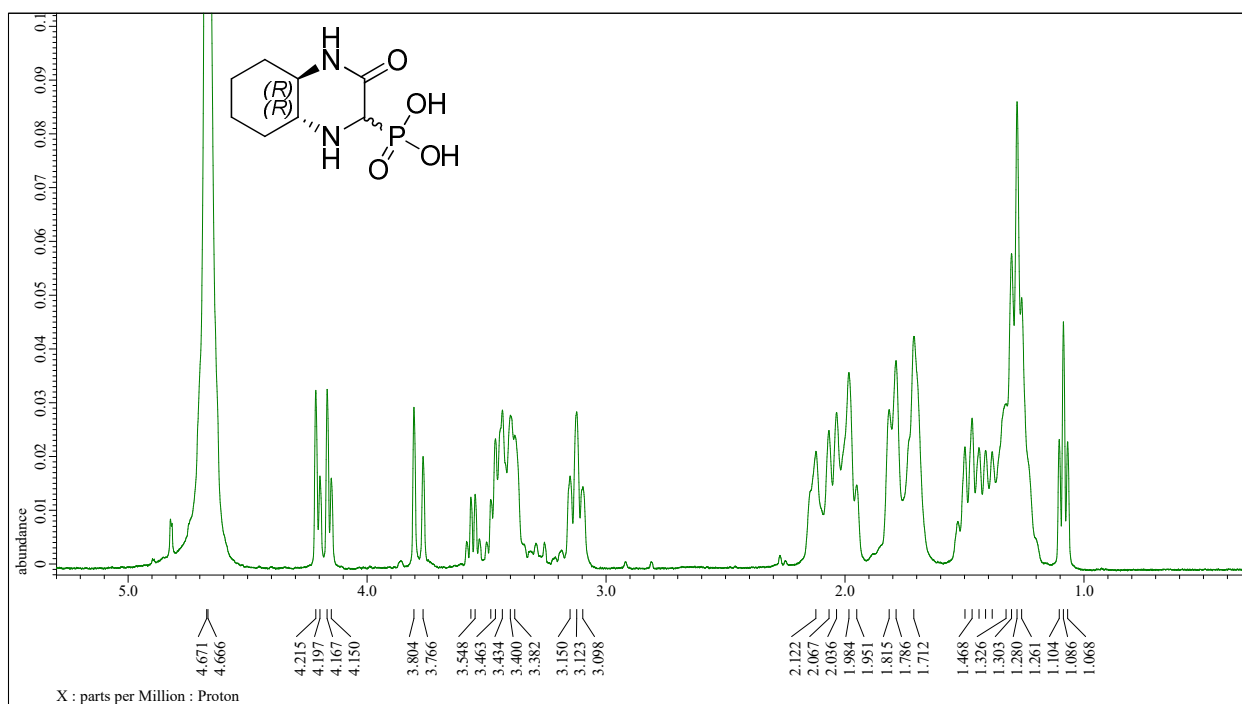


(b)



(c)

Figure S8. (a) ^1H NMR, (b) ^{13}C NMR and (c) ^{31}P NMR spectra of (4-((3*aR*,8*aR*)-2,2-dimethyl-6-oxido-4,4,8,8-tetraphenyltetrahydro-[1,3]dioxolo[4,5-*e*][1,3,2]dioxaphosphepin-6-yl))-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]decan 2g.



(a)

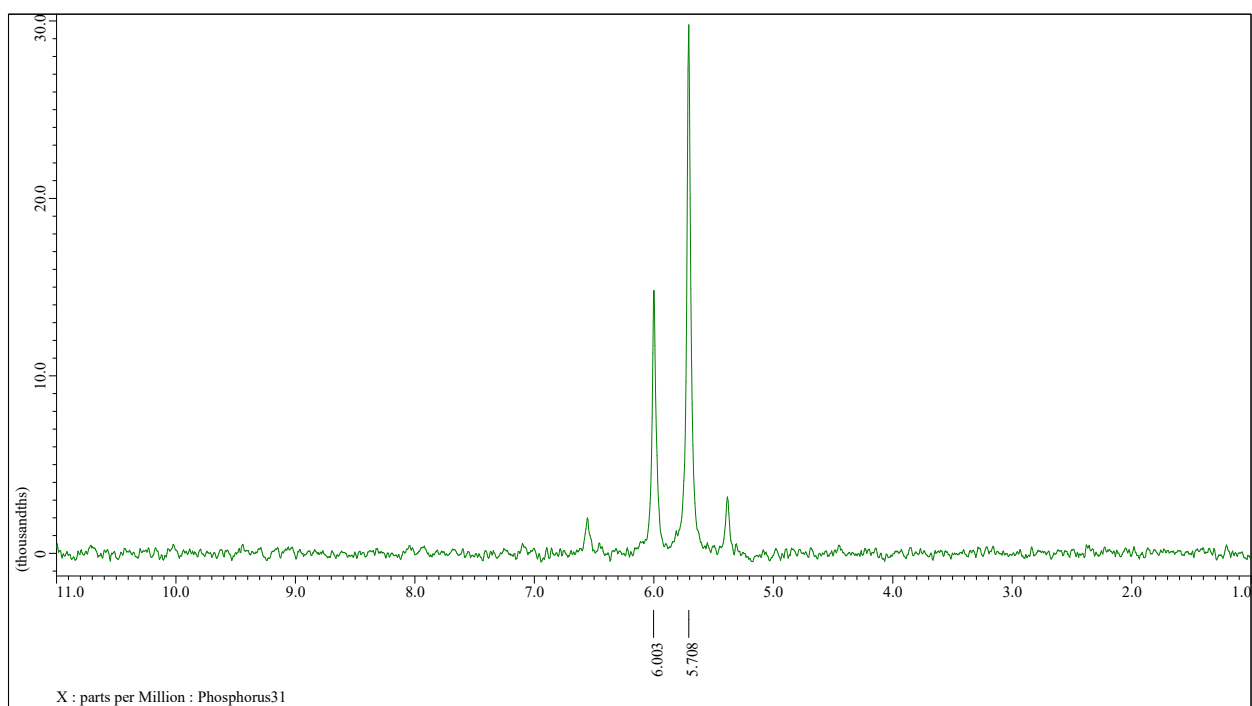
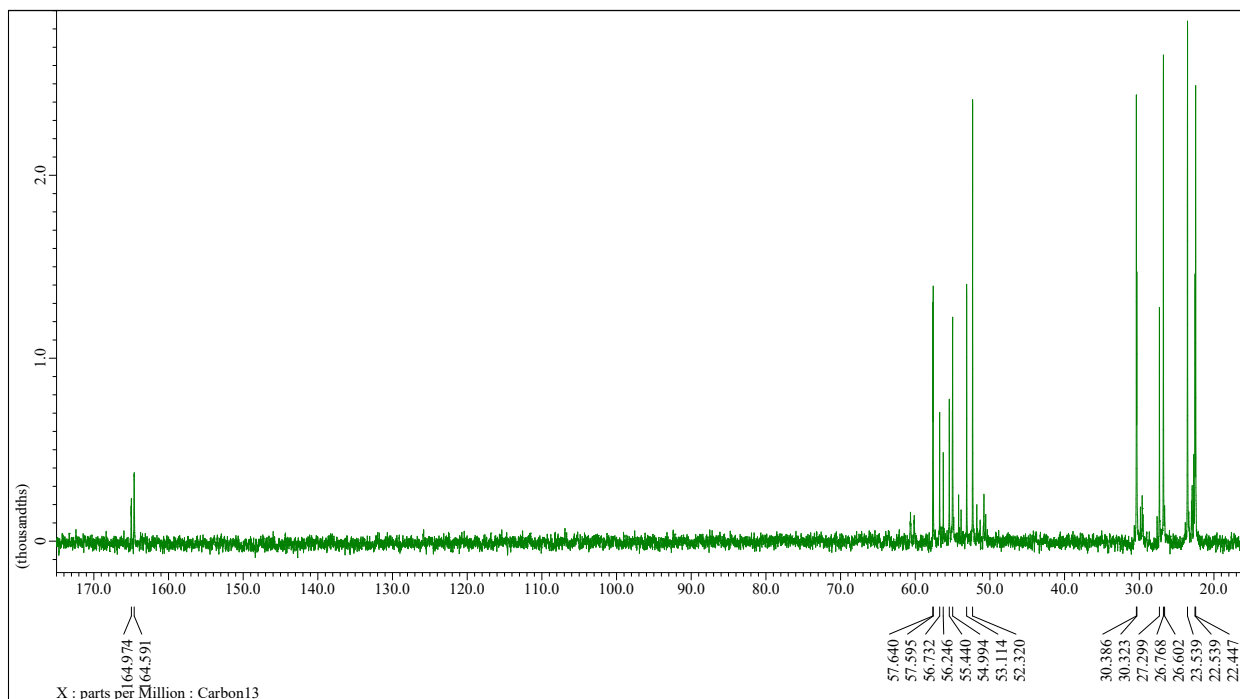
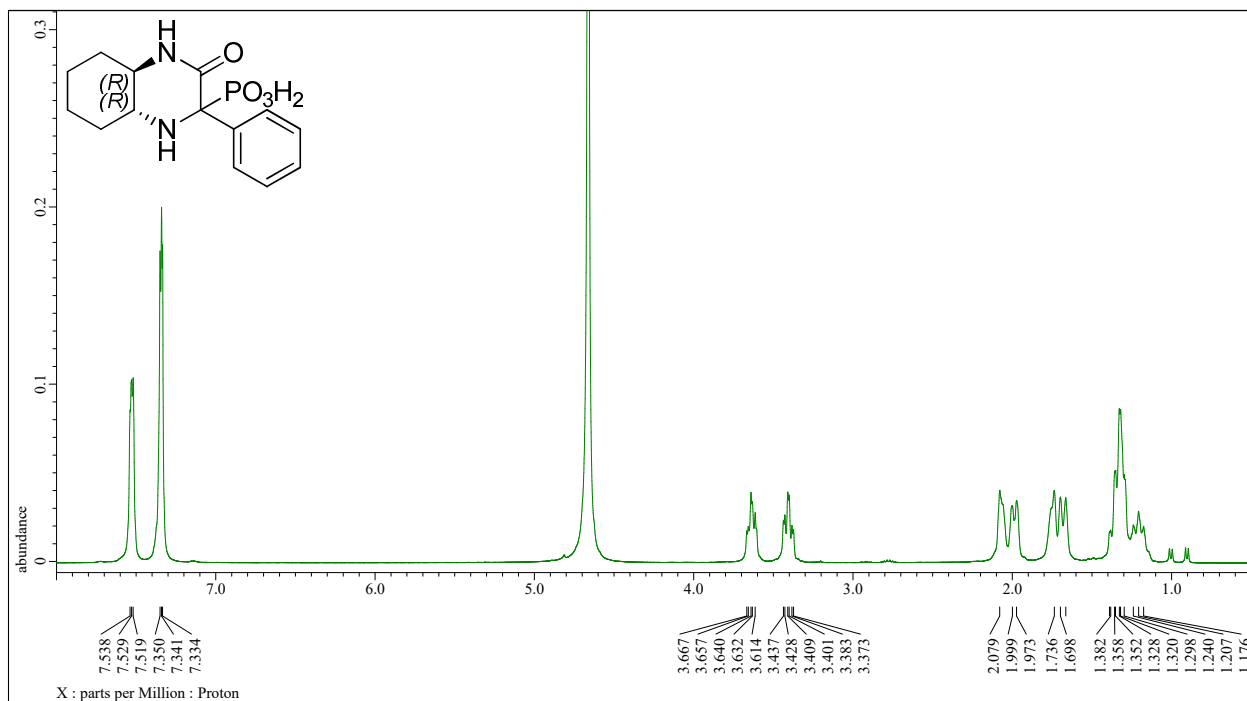
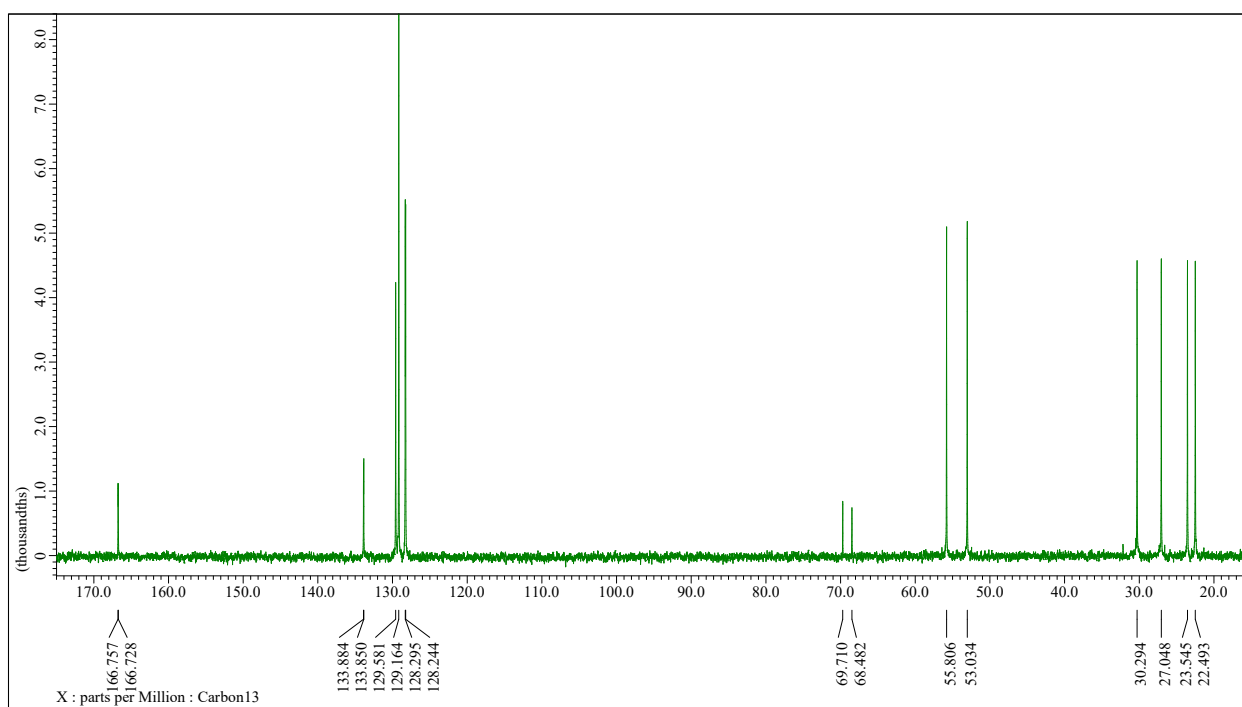


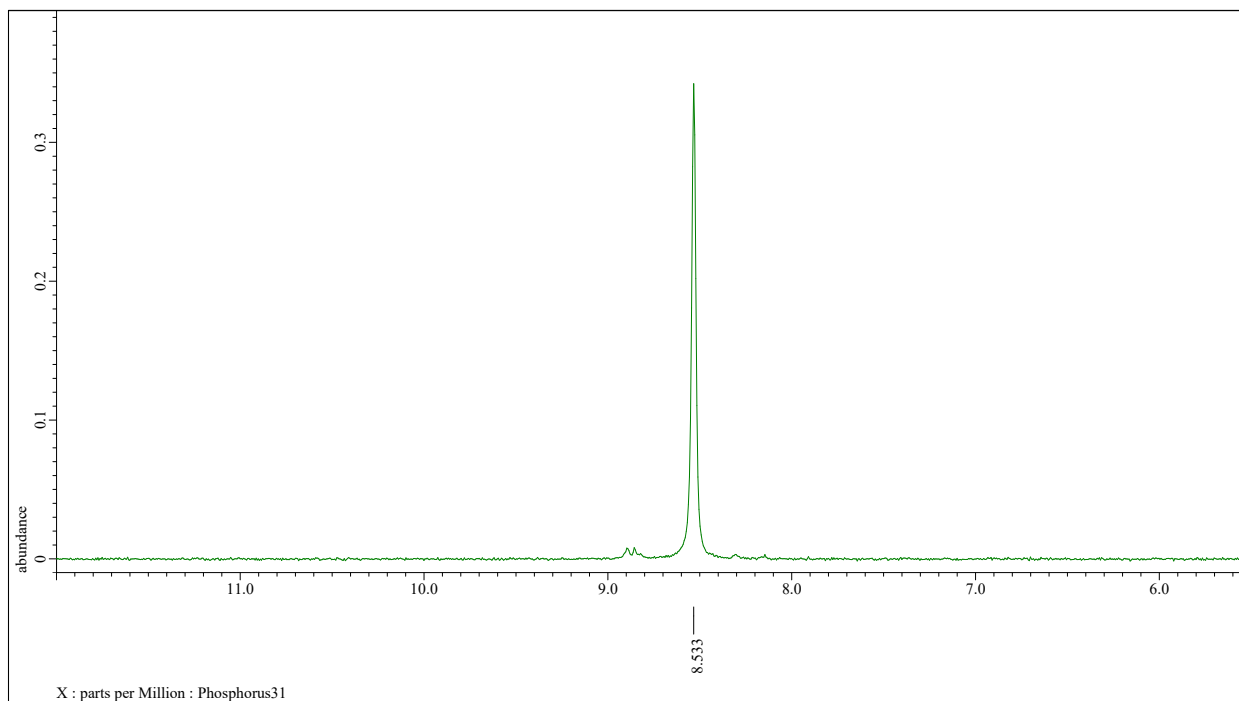
Figure S9. (a) ^1H NMR, (b) ^{13}C NMR and (c) ^{31}P NMR spectra of [(1R,6R)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid 3a.



(a)



(b)



(c)

Figure S10. (a) ^1H NMR, (b) ^{13}C NMR and (c) ^{31}P NMR spectra of [4-phenyl-(1*R*,6*R*)-3-oxo-2,5-diazabicyclo[4.4.0]dec-4-yl]-phosphonic acid 3b.



© 2020 by the authors. Submitted for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).