

## Supporting Information

### How Intramolecular Hydrogen Bonding (IHB) Controls the C—ON Bond Homolysis in Alkoxyamines.

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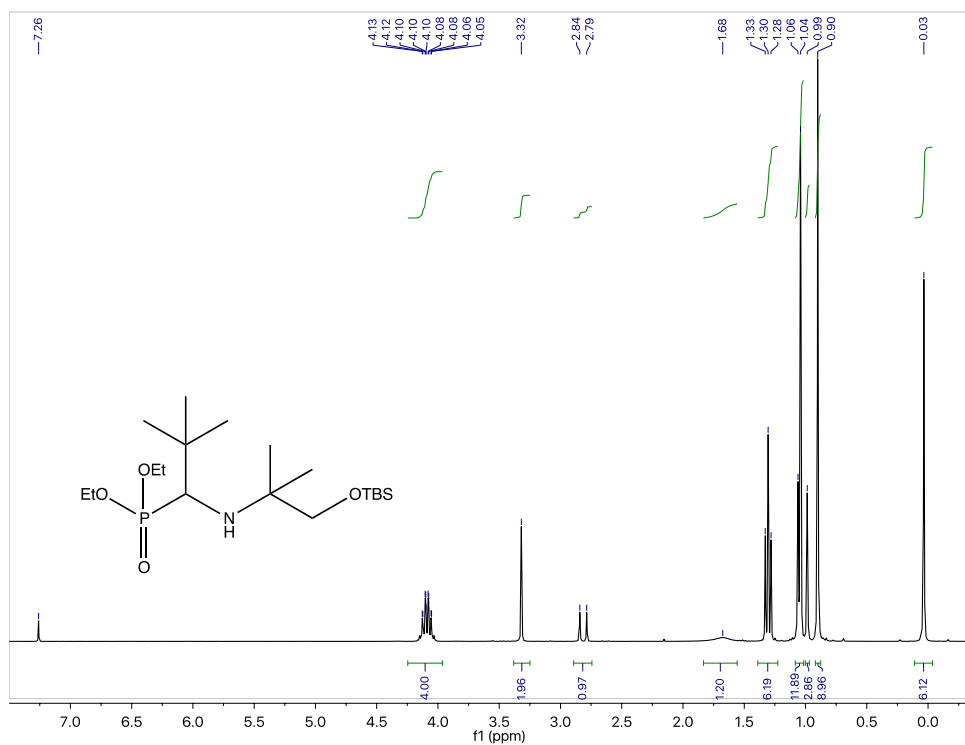
E-mail: sylvain.marque@univ-amu.fr, g.audran@univ-amu.fr

\* to whom correspondence should be sent

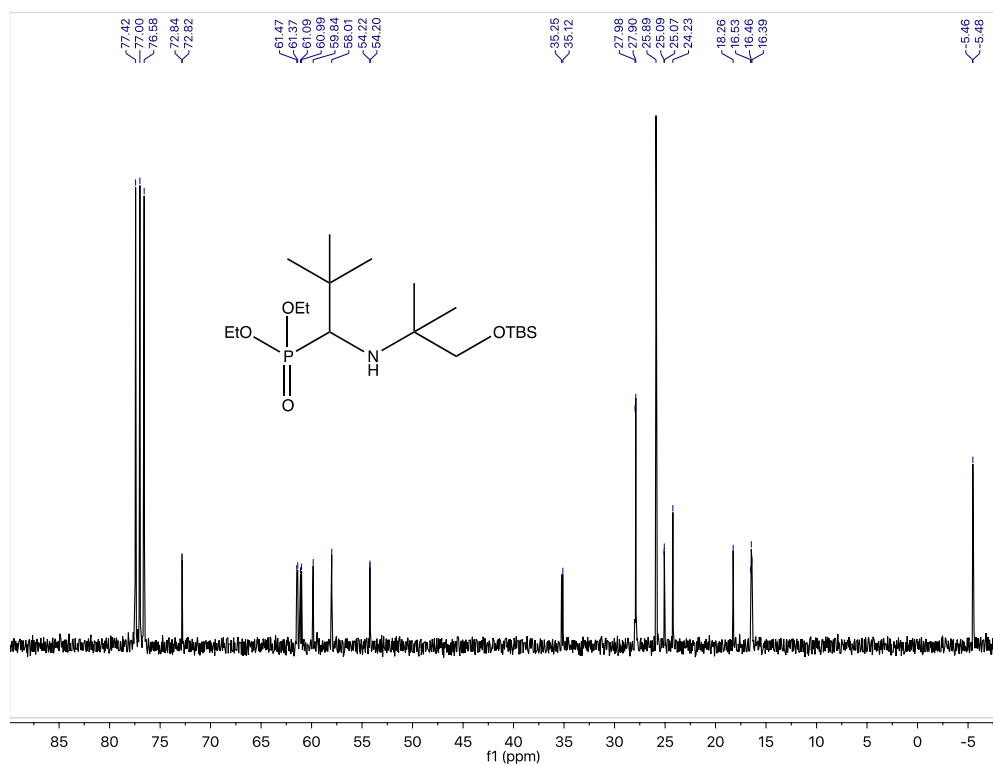
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Diethyl (1-((1-((tert-butyldimethylsilyl)oxy)-2-methylpropan-2-yl)amino)-2,2-dimethylpropyl) phosphonate (**2b**)

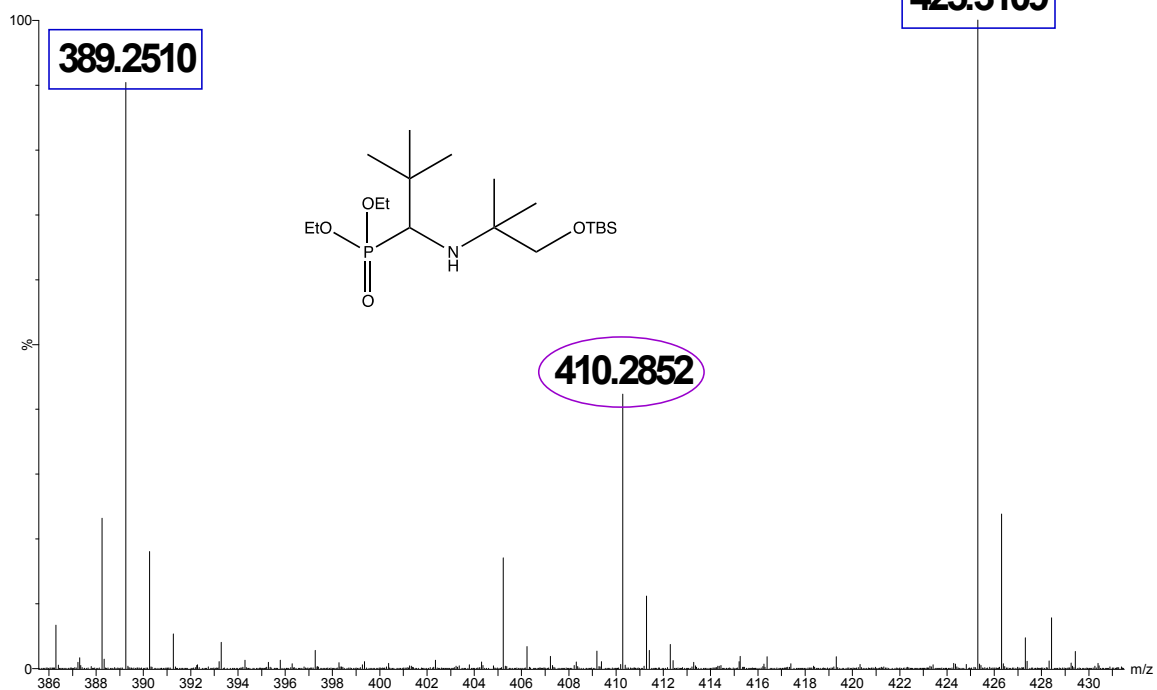
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):



**2b**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):



**2b** HRMS

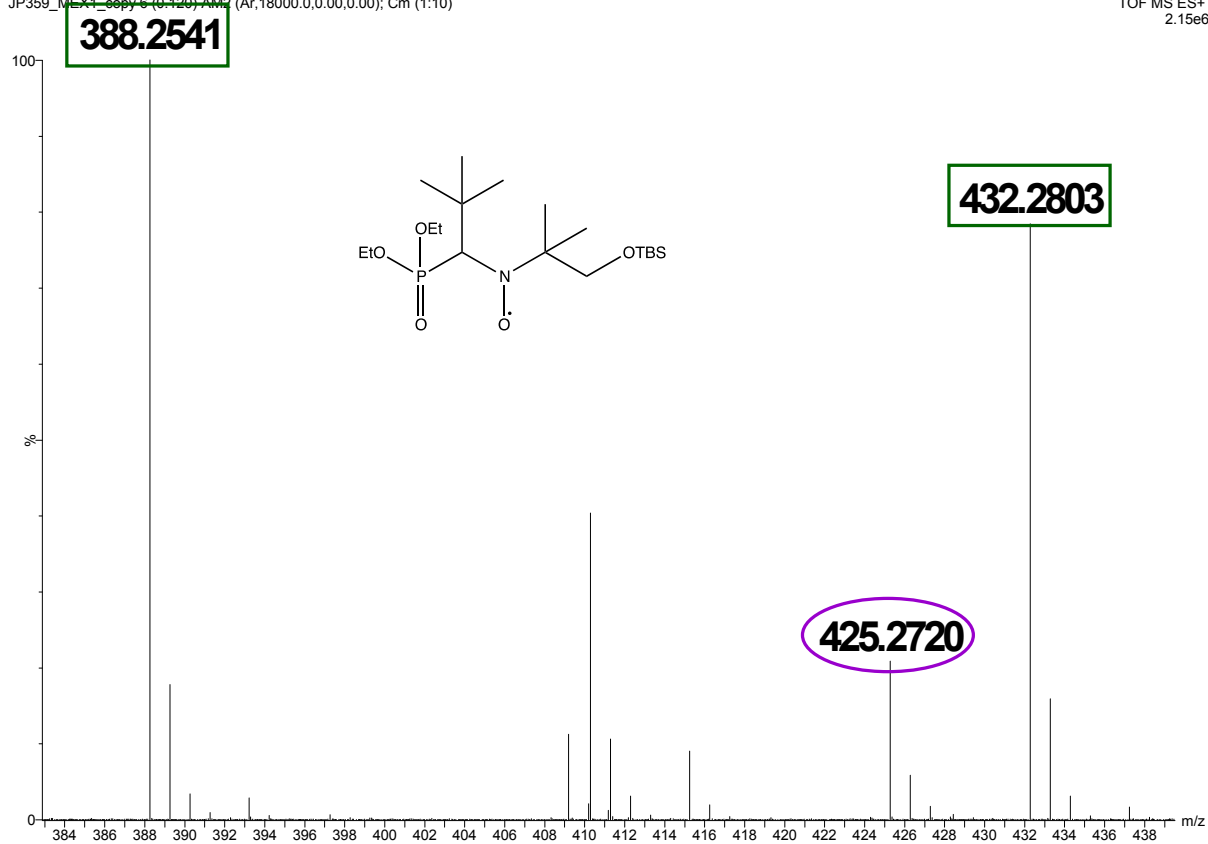


*1-(Diethoxyphosphoryl)-2,2-dimethylpropyl 2-(tert-butyl dimethylsilyloxy)-1,1-dimethylethyl Nitroxide (2•)*

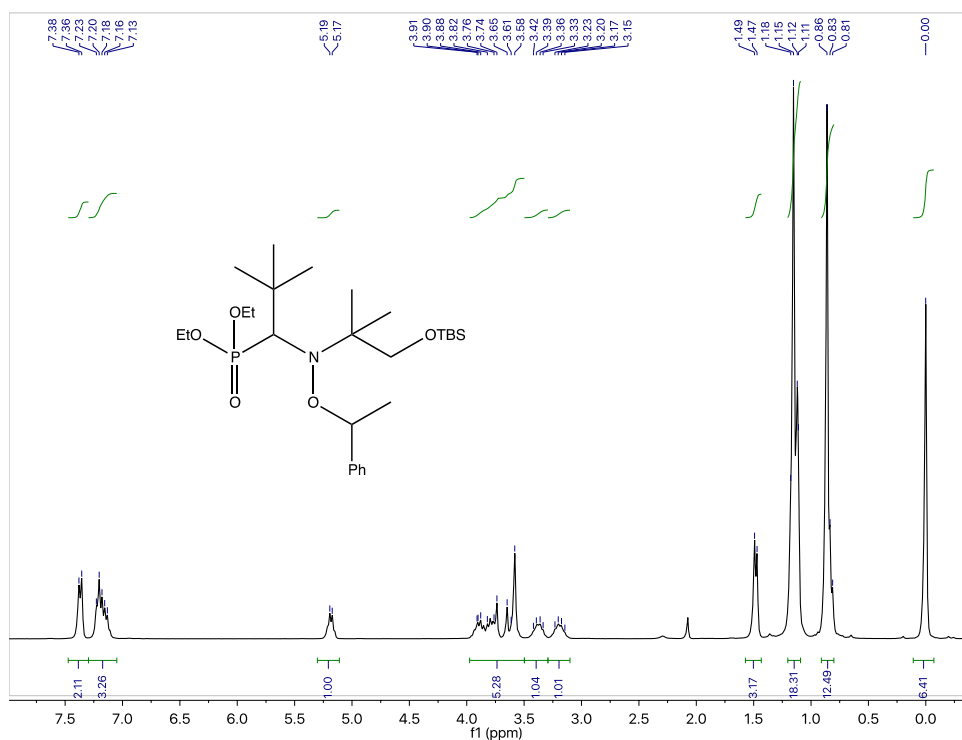
2• HRMS

JP359\_MEX1\_copy 6 (0.120).AM2 (Ar,18000.0,0.00,0.00); Cm (1:10)

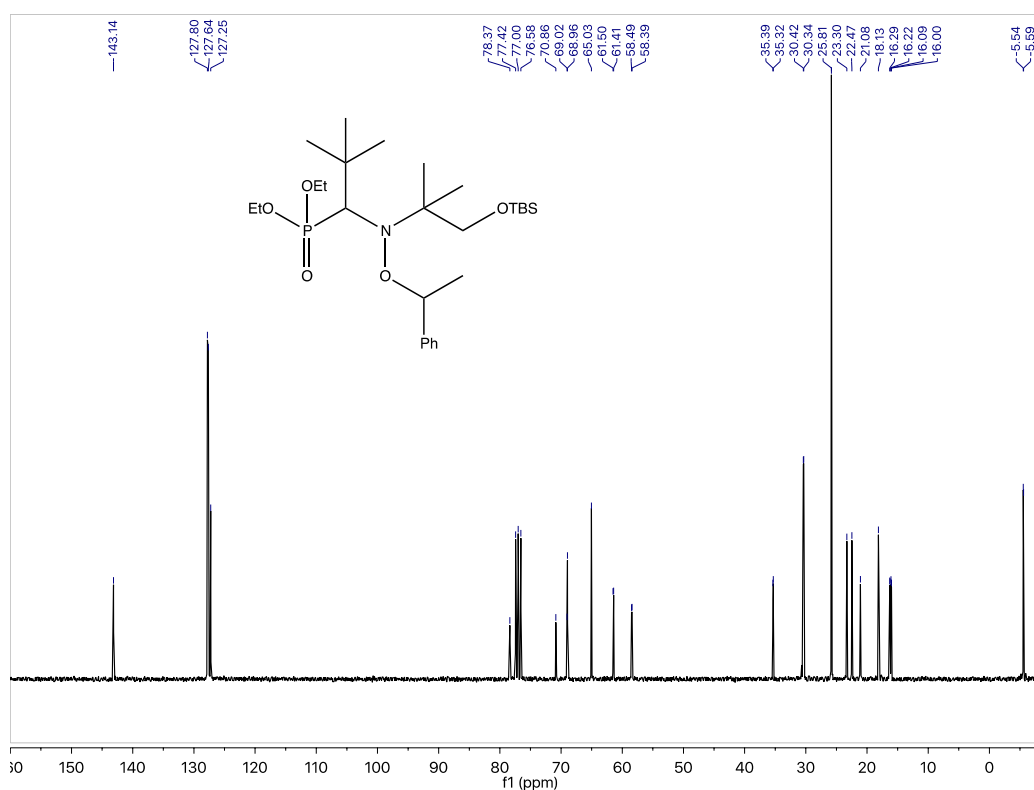
TOF MS ES+  
2.15e6



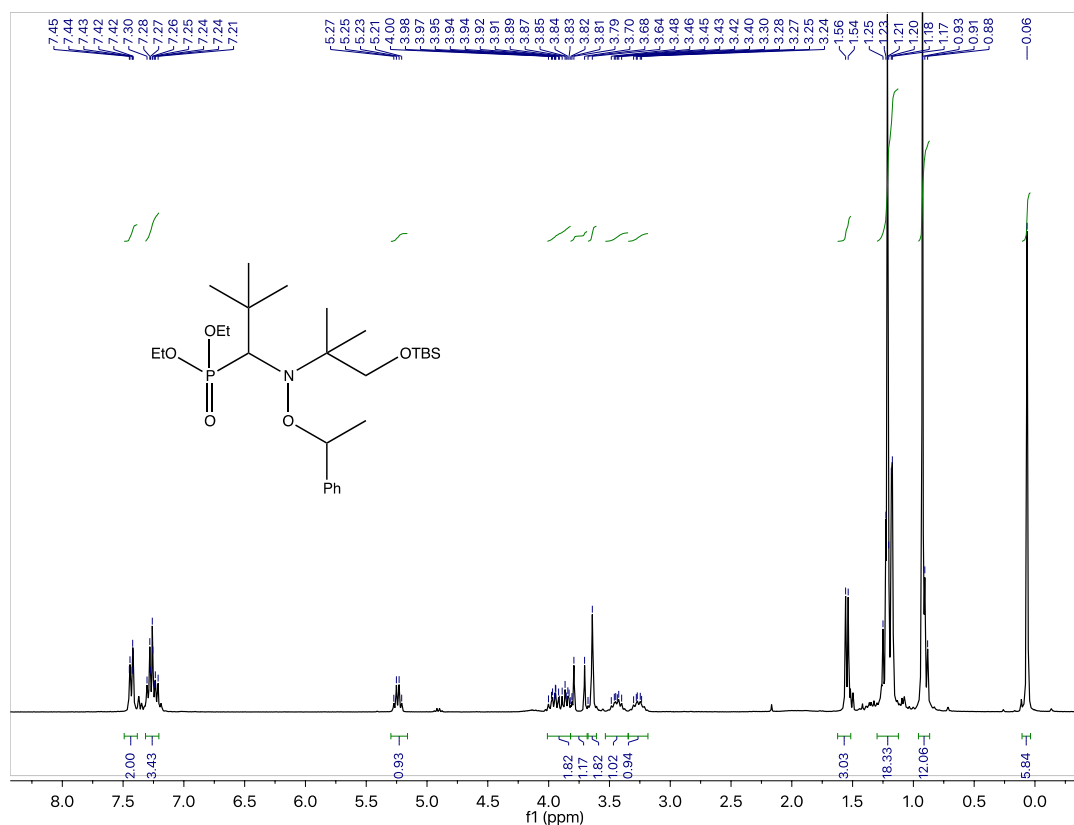
Diethyl(1-((1-((tert-butyl dimethylsilyl)oxy)-2-methylpropan-2-yl)(1-phenylethoxy)amino)-2,2-dimethylpropyl)phosphonate (**2, 2', 2''**)  
*RS/SR-2* <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz):



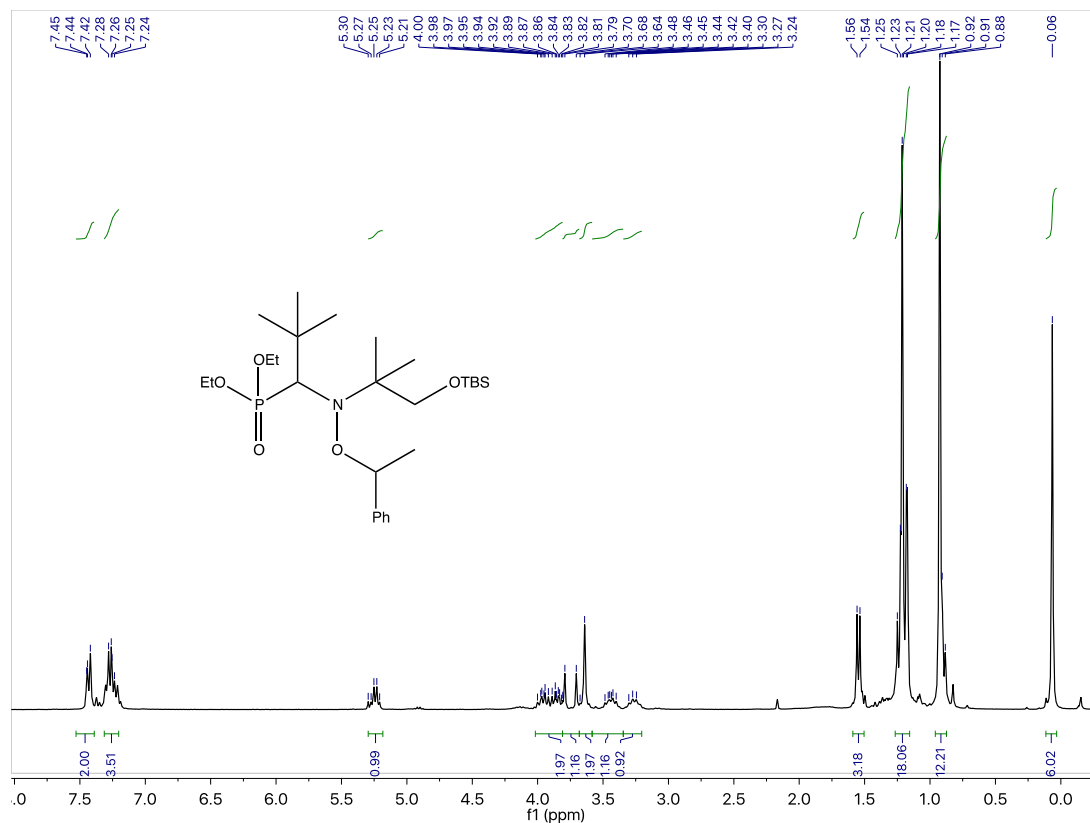
*RS/SR-2* <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz):



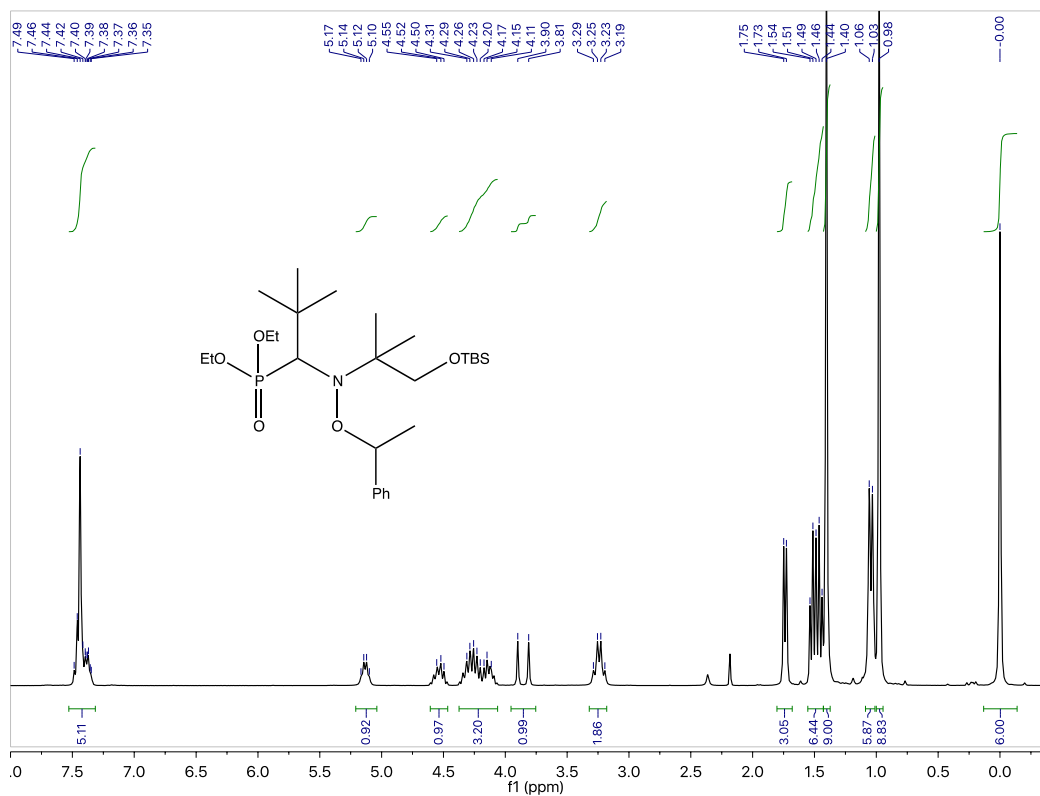
***RS/SR-2'*** <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz):



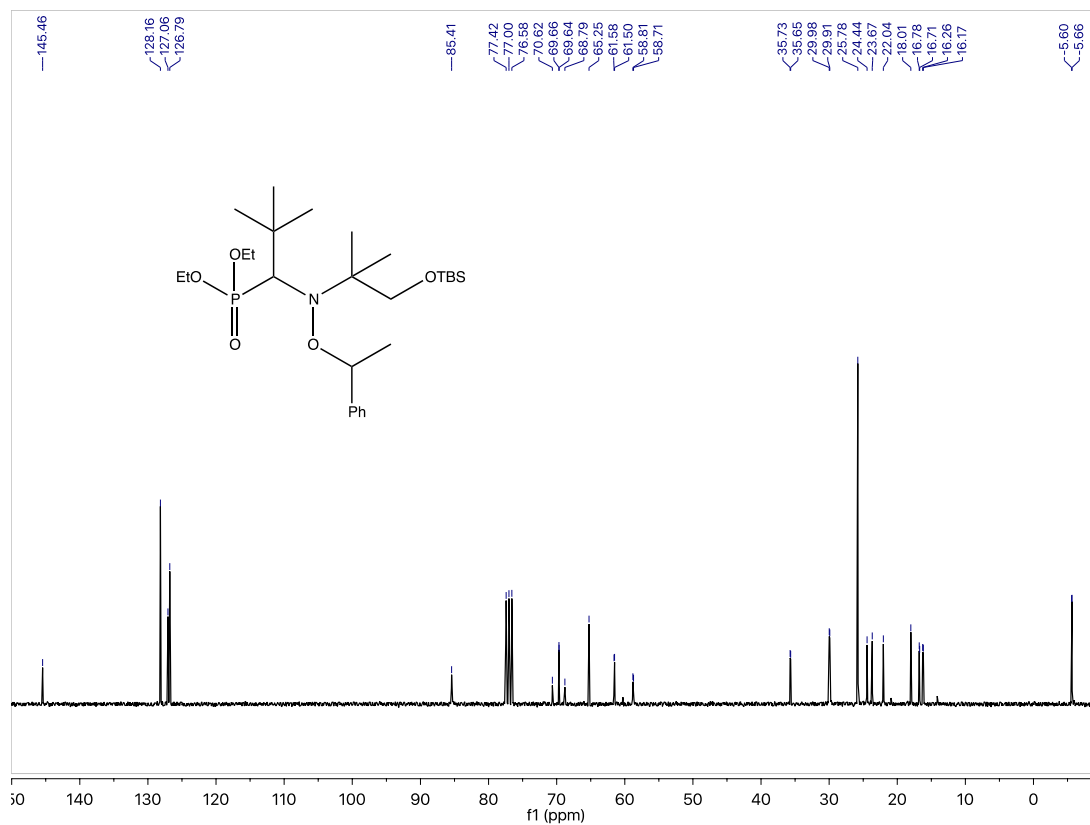
**RS/SR-2''** <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz):



***RR/SS-2***  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):

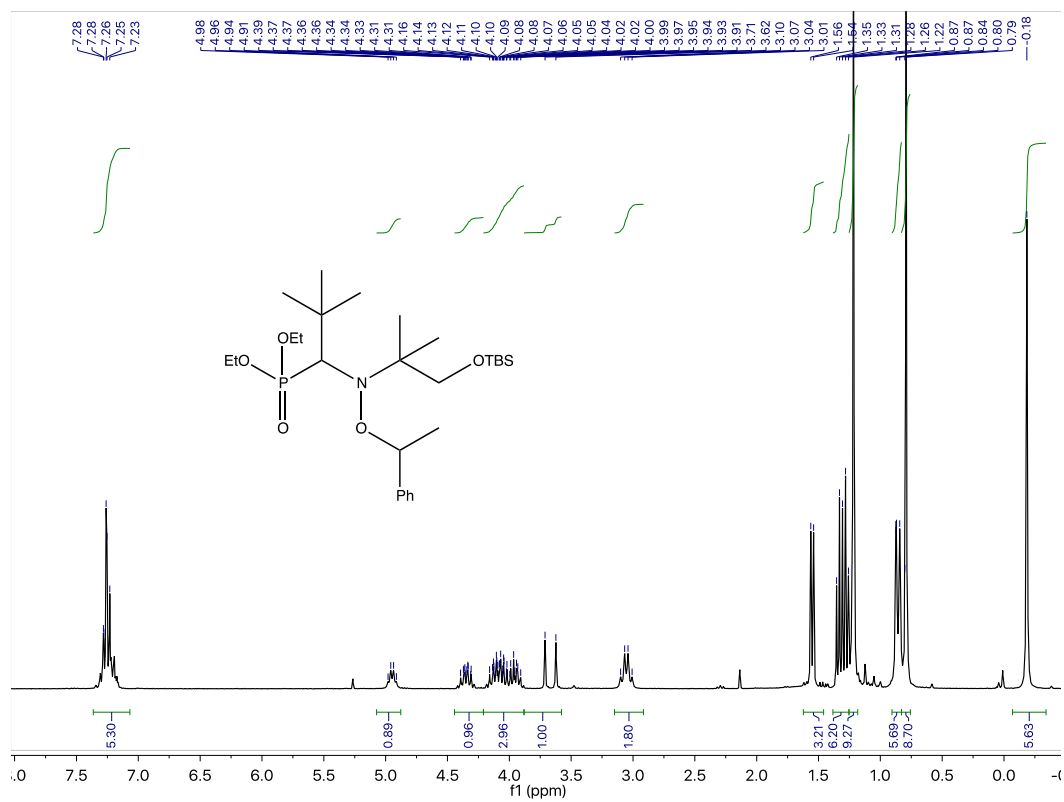


***RR/SS-2***  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):

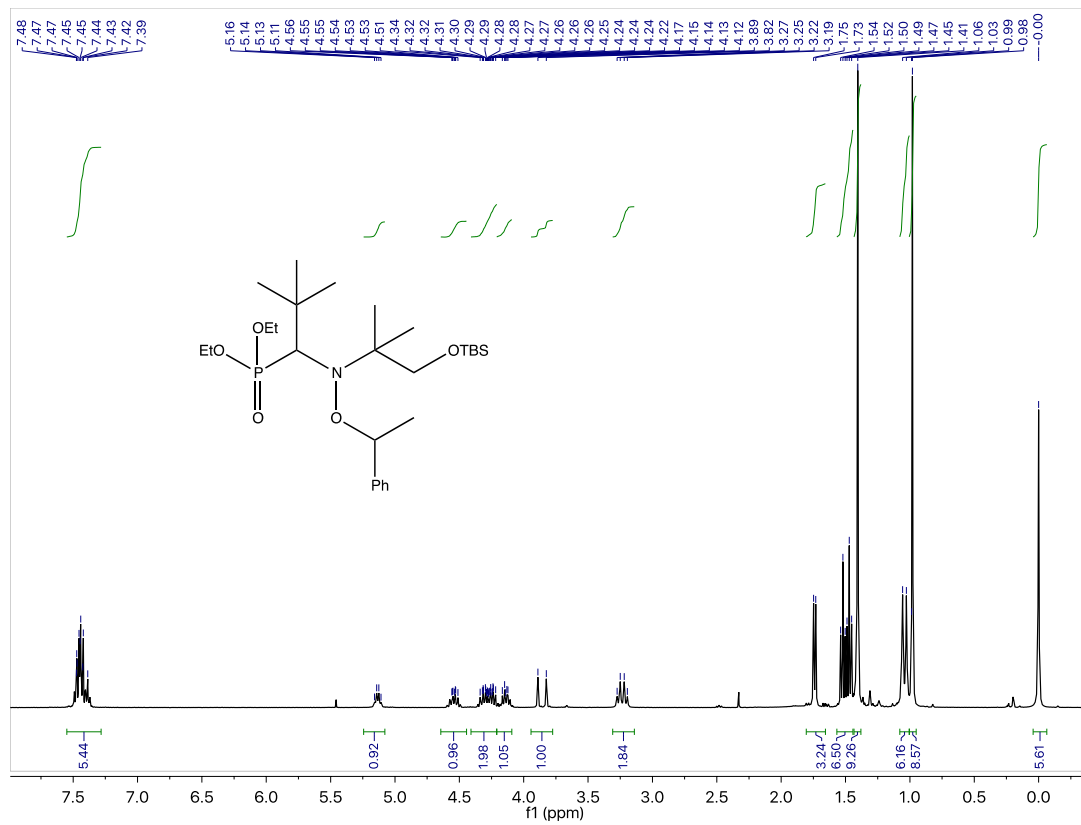




***RR/SS-2'*** <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz):



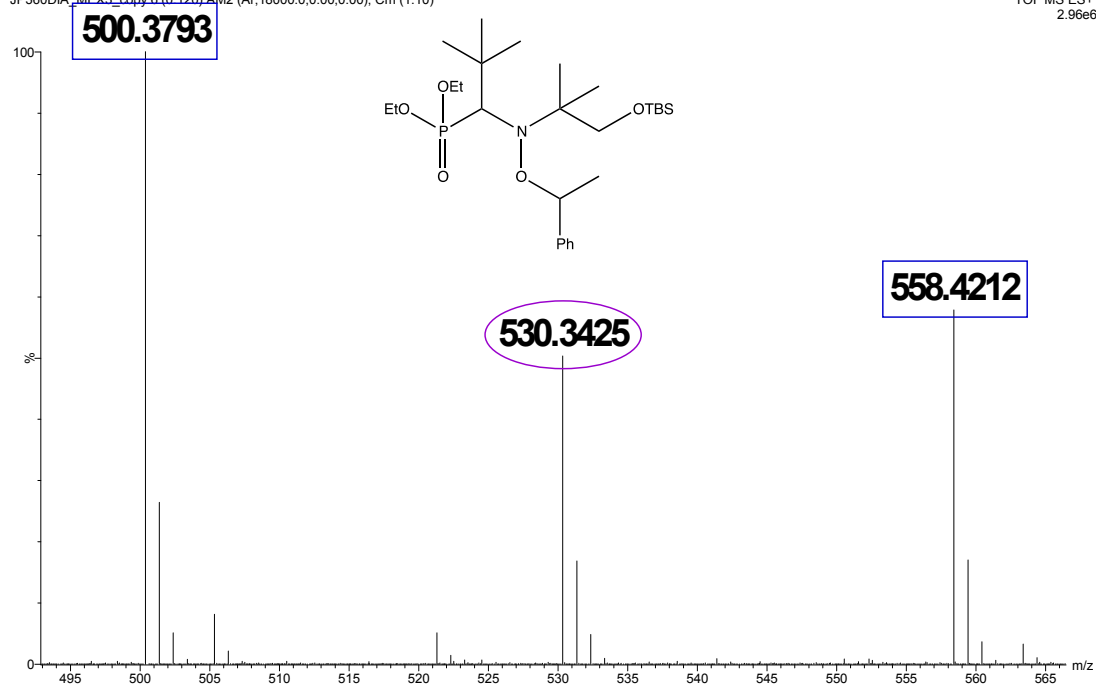
*RR/SS-2''*  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):



# RS/SR-2 and RR/SS-2 mixture HRMS

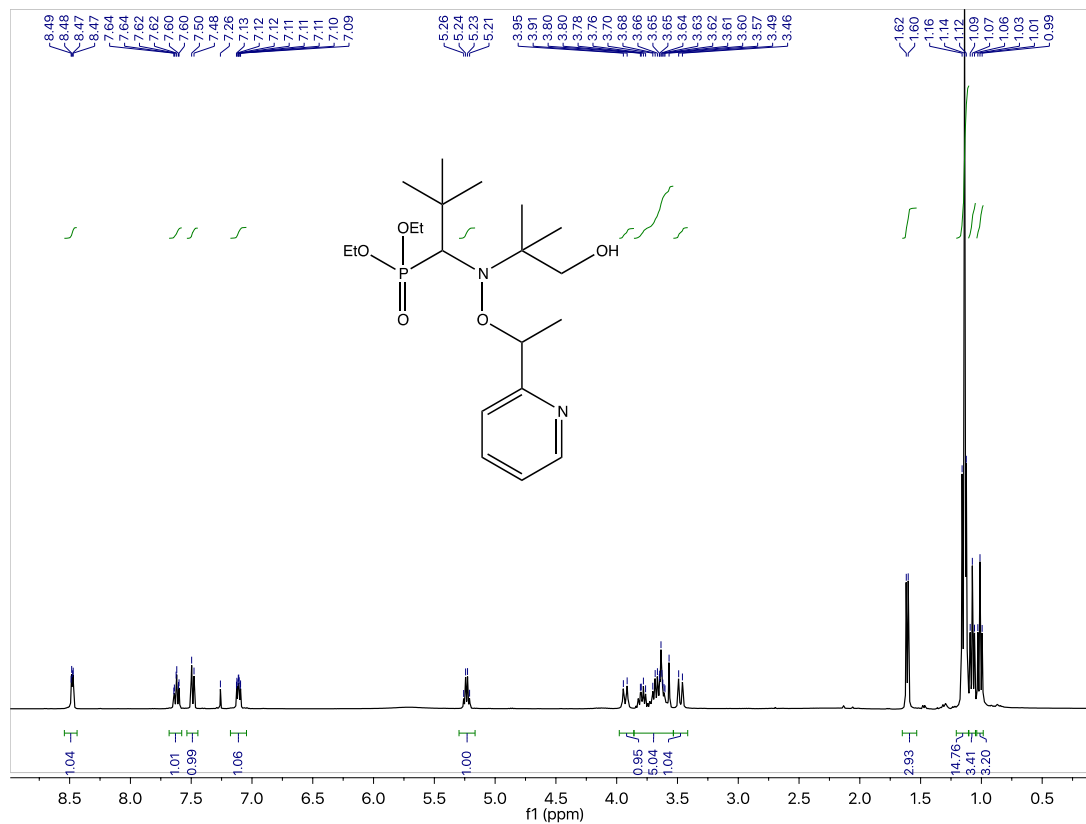
JP360DIA\_MEX3\_copy.6(0.120).AM2 (Ar,18000.0,0.00,0.00); Cm (1:10)

TOF MS ES+  
2.96e6

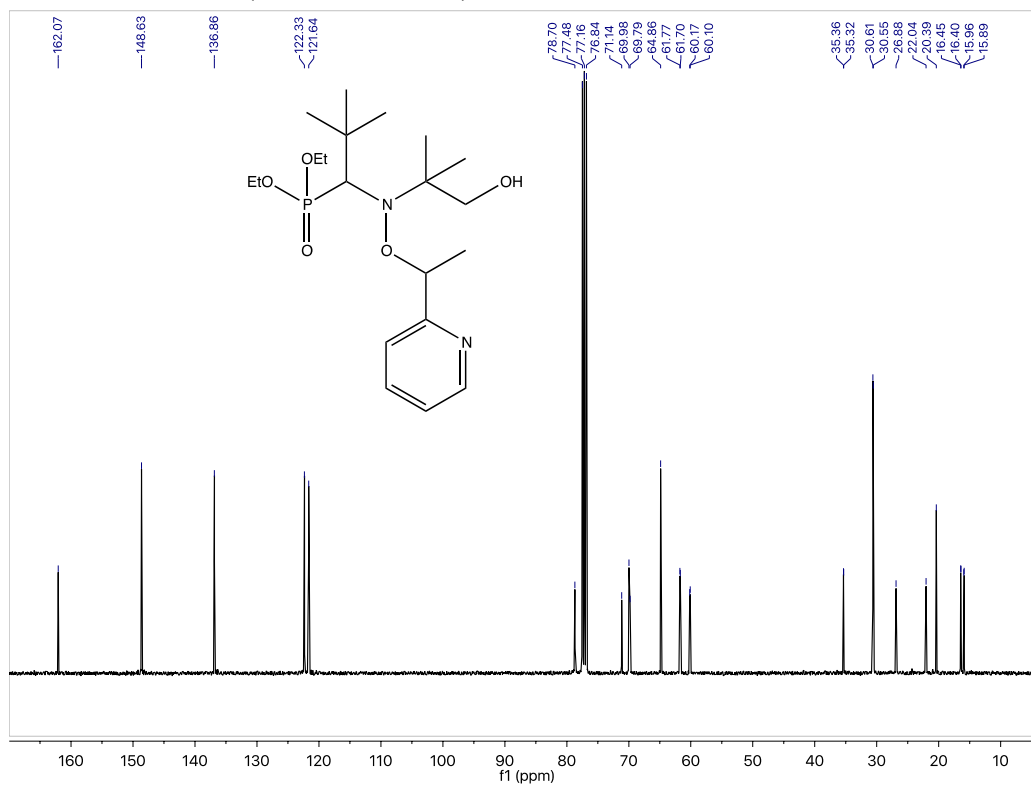


*Diethyl-(1-((1-hydroxy-2-methylpropan-2-yl)(1-(pyridin-2-yl)ethoxy)amino)-2,2-dimethylpropyl) phosphonate (4).*

**RS/SR-4**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):



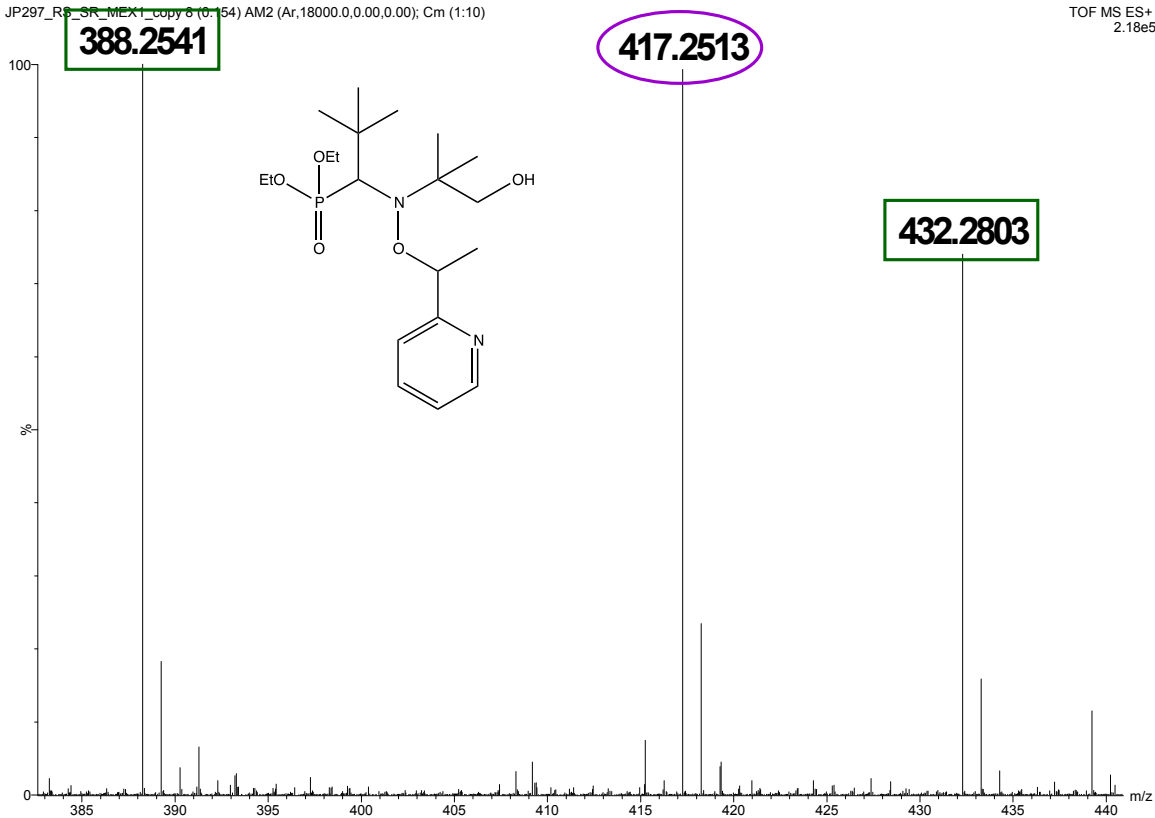
**RS/SR-4**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):



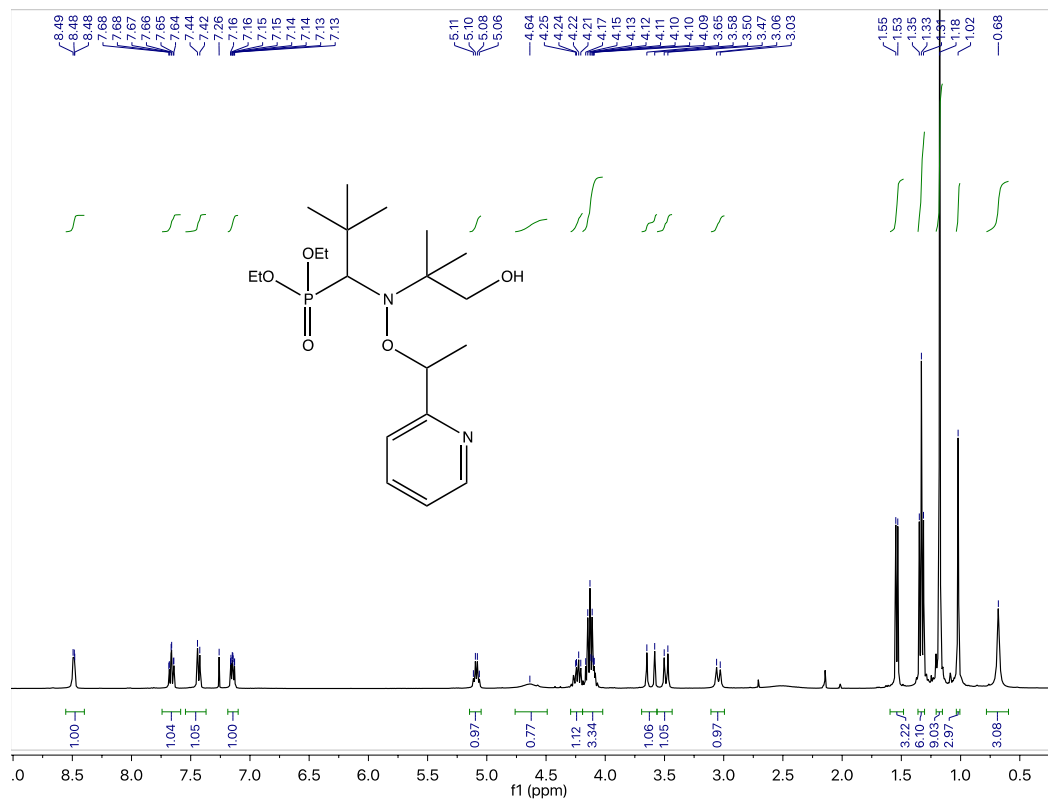
RS/SR-4 HRMS

JP297\_R6\_SR\_MEX1\_copy 8 (0.64) AM2 (Ar,18000.0,0.00,0.00); Cm (1:10)

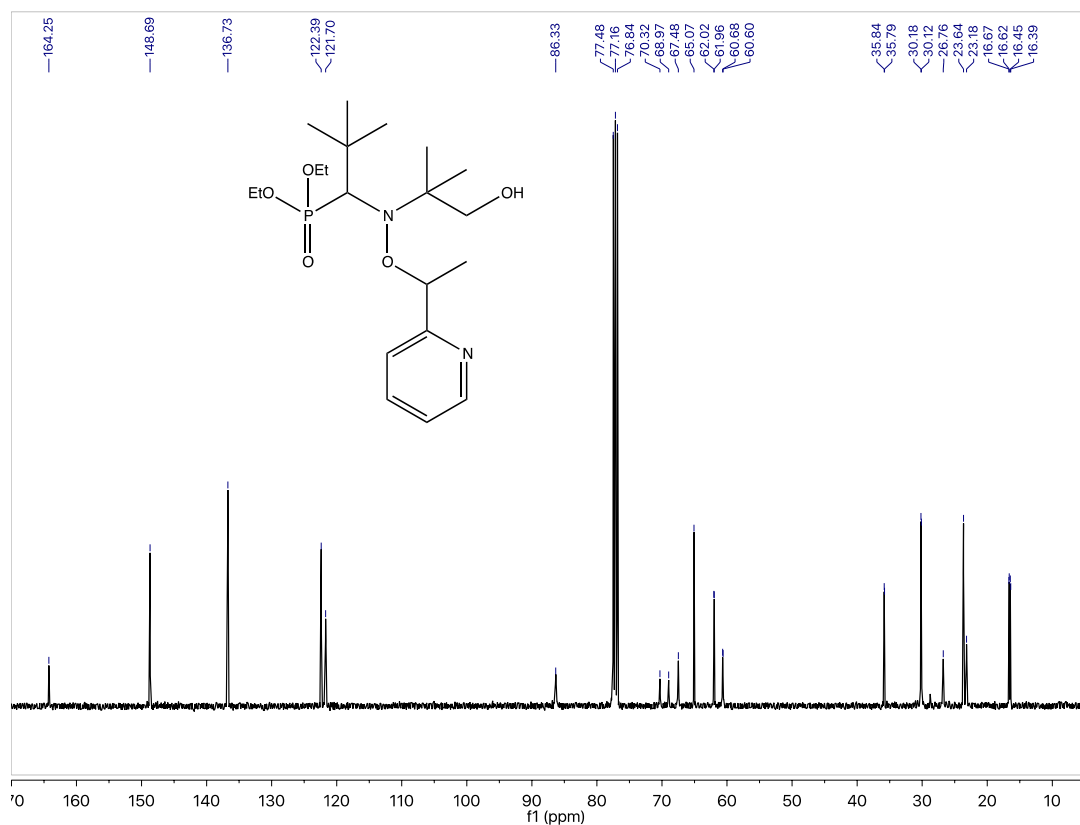
TOF MS ES+  
2.18e5



***RR/SS-4***  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):



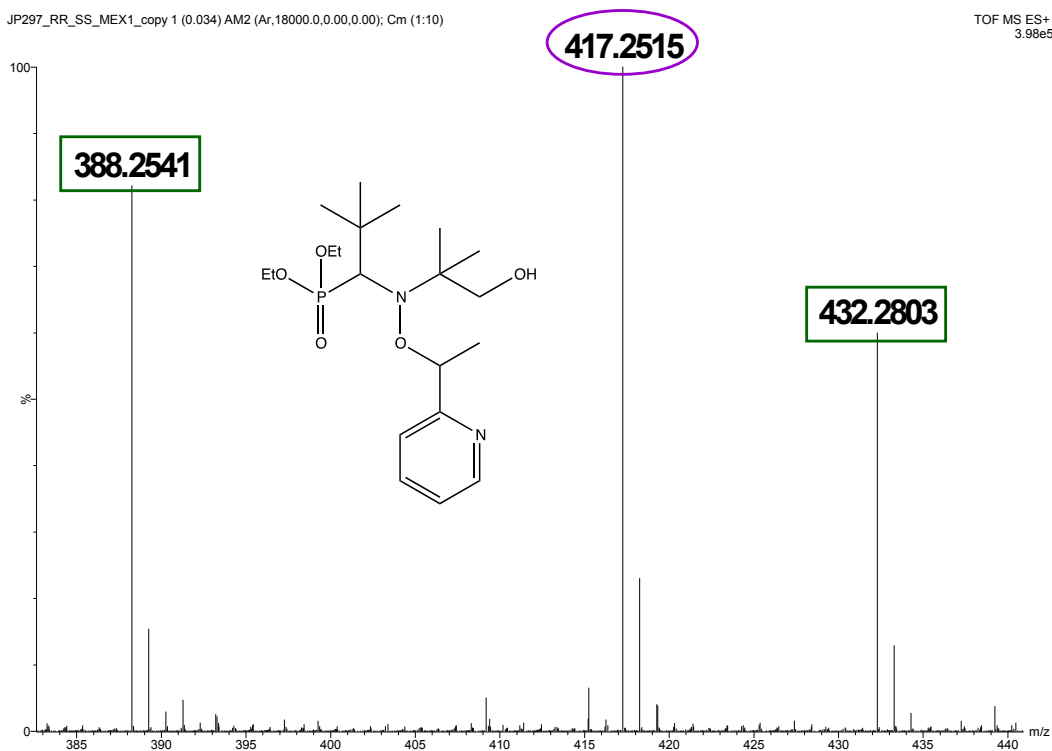
***RR/SS-4***  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):



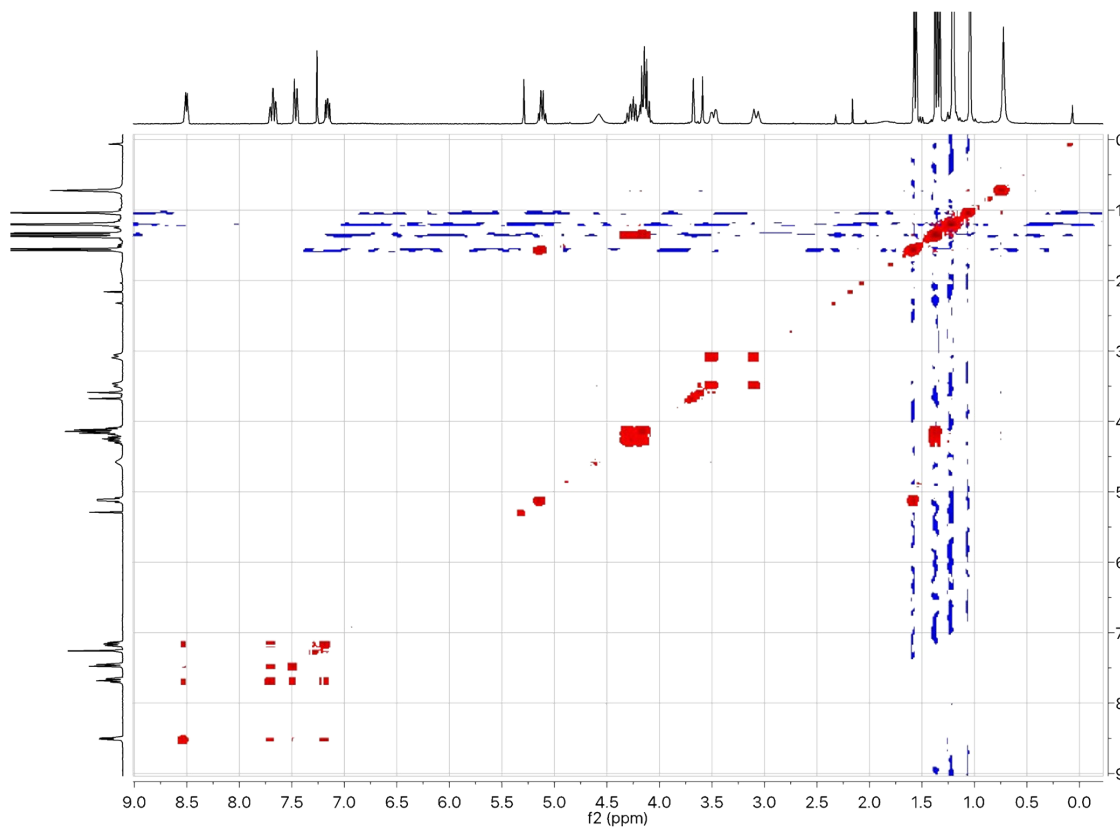
# RR/SS-4 HRMS

JP297\_RR\_SS\_MEX1\_copy 1 (0.034) AM2 (Ar,18000.0,0.00,0.00); Cm (1:10)

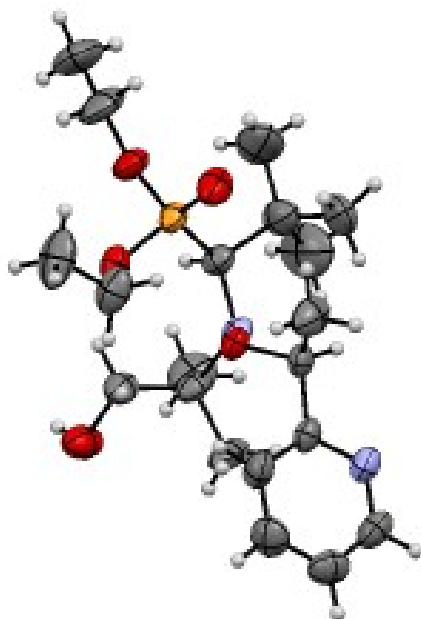
TOF MS ES+  
3.98e5



# RR/SS-4 COSY



*RR/SS-4* : The ellipsoid contour percent is given at 50% for the ORTEP plot.



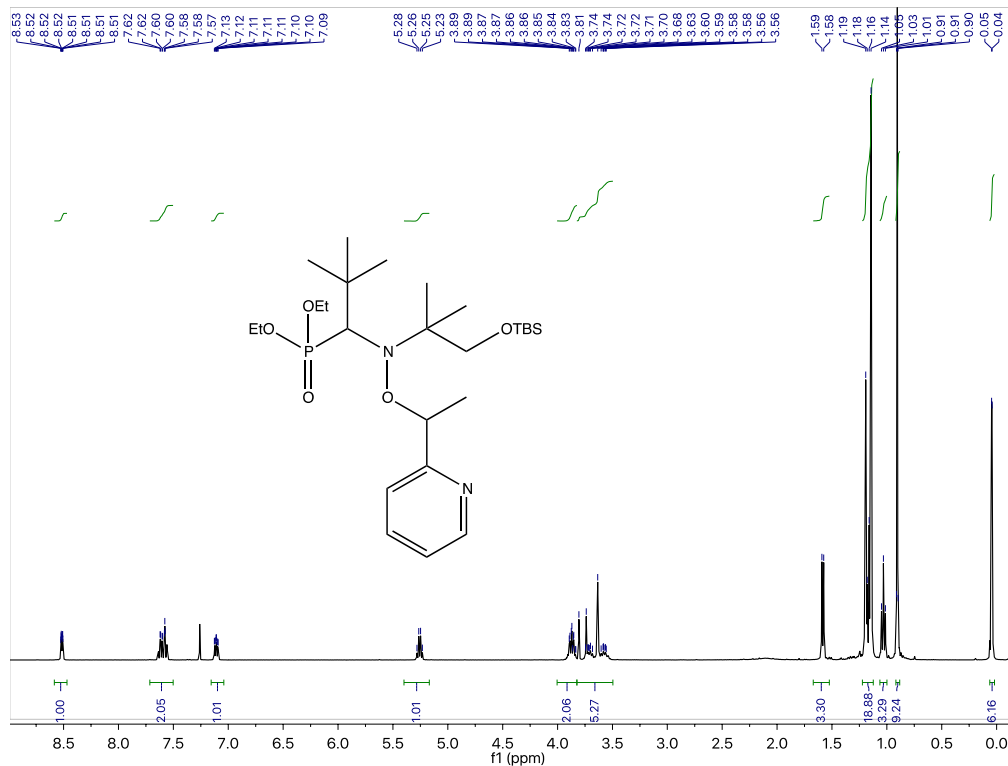
**Table 1SI.** XRD data for *RR/SS-4*

Empirical formula	C <sub>20</sub> H <sub>37</sub> N <sub>2</sub> O <sub>5</sub> P	$\mu/\text{mm}^{-1}$	0.148
Formula weight	416.48	F(000)	904.0
Temperature/K	293	Crystal size/mm <sup>3</sup>	0.34 × 0.2 × 0.08
Crystal system	monoclinic	Radiation	MoK $\alpha$ ( $\lambda = 0.71073$ )
Space group	P2 <sub>1</sub> /c	2 $\Theta$ range for data collection/°	6.738 to 56.766
a/Å	14.4884(6)	Index ranges	-19 ≤ h ≤ 18, -15 ≤ k ≤ 15, -17 ≤ l ≤ 16
b/Å	12.0955(4)	Reflections collected	18820
c/Å	14.1006(6)	Independent reflections	5038 [R <sub>int</sub> = 0.0299, R <sub>sigma</sub> = 0.0274]
$\alpha$ /°	90	Data/restraints/parameters	5038/0/262
$\beta$ /°	108.748(5)	Goodness-of-fit on F <sup>2</sup>	1.035
$\gamma$ /°	90	Final R indexes [I >= 2 $\sigma$ (I)]	R <sub>1</sub> = 0.0489, wR <sub>2</sub> = 0.1227
Volume/Å <sup>3</sup>	2339.94(17)	Final R indexes [all data]	R <sub>1</sub> = 0.0700, wR <sub>2</sub> = 0.1359
Z	4	Largest diff. peak/hole / e Å <sup>-3</sup>	0.28/-0.28
$\rho_{\text{calc}}/\text{g}/\text{cm}^3$	1.182		

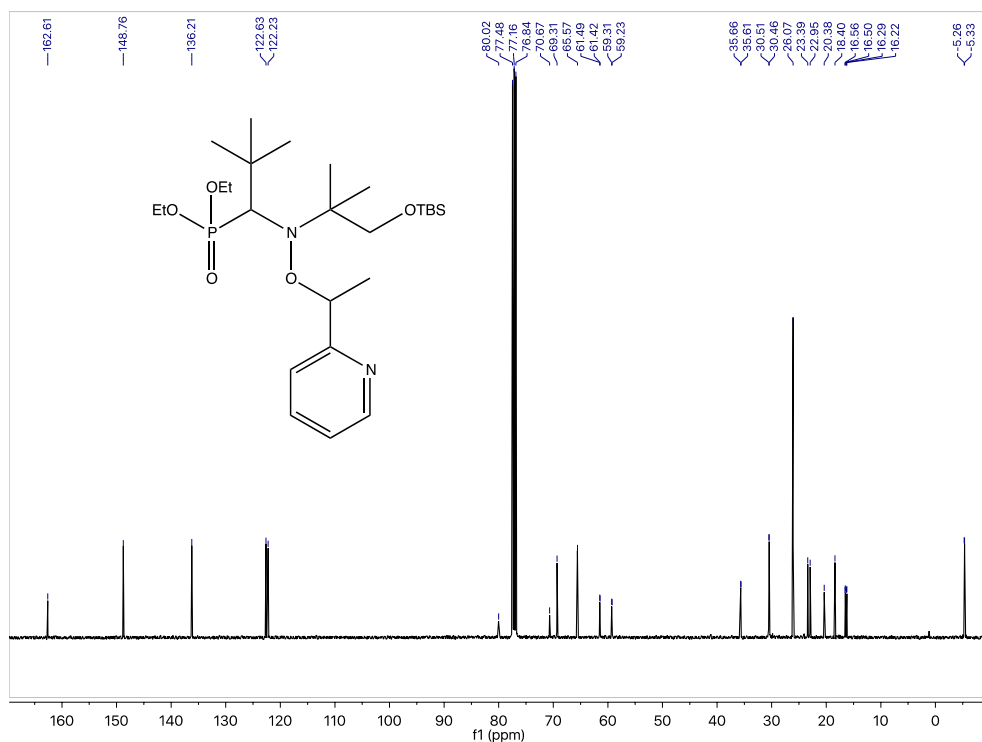


Diethyl ((R)-1-((1-hydroxy-2-methylpropan-2-yl)((S)-1-(pyridin-2-yl)ethoxy)amino)-2,2-dimethylpropyl)phosphonate (*RS/SR*-5).

*RS/SR*-5 <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz):

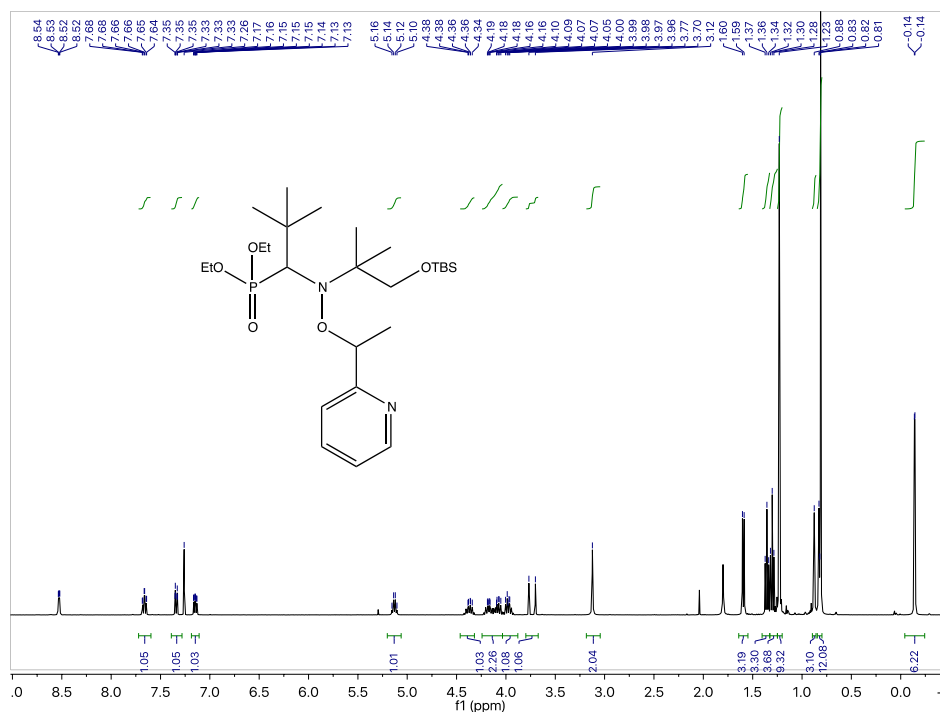


*RS/SR*-5 <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz):

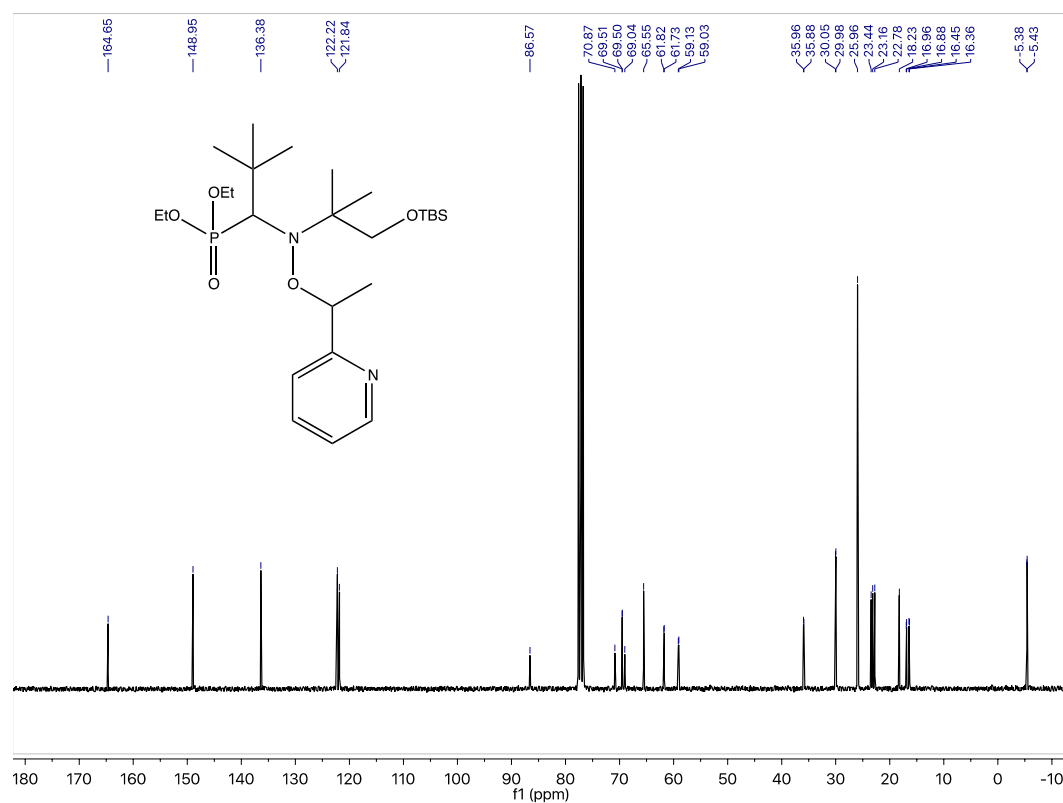


Diethyl((R)-1-((1-hydroxy-2-methylpropan-2-yl)((R)-1-(pyridin-2-yl)ethoxy)amino)-2,2-dimethylpropyl)phosphonate (RR/SS-5).

RR/SS-5 <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz):



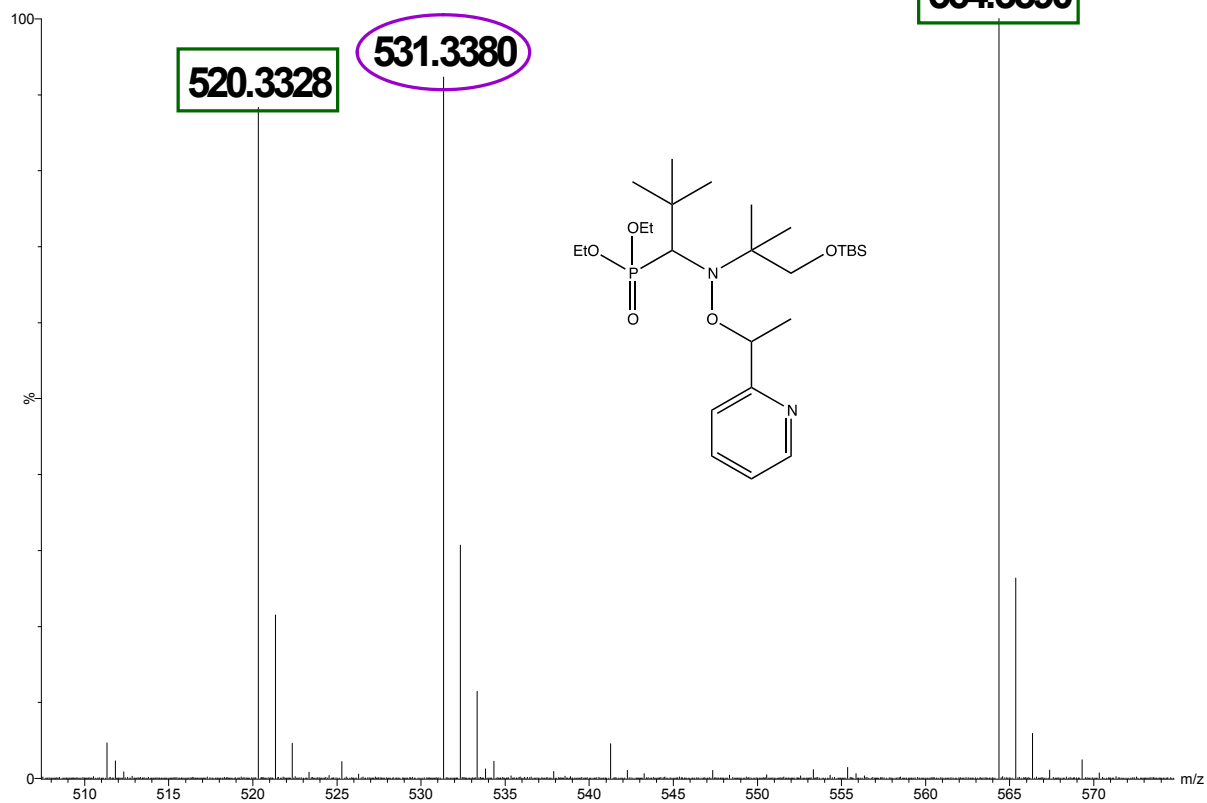
RR/SS-5 <sup>13</sup>C NMR (CDCl<sub>3</sub>, 101 MHz):



# RS/SR-5 and RR/SS-5 mixture HRMS

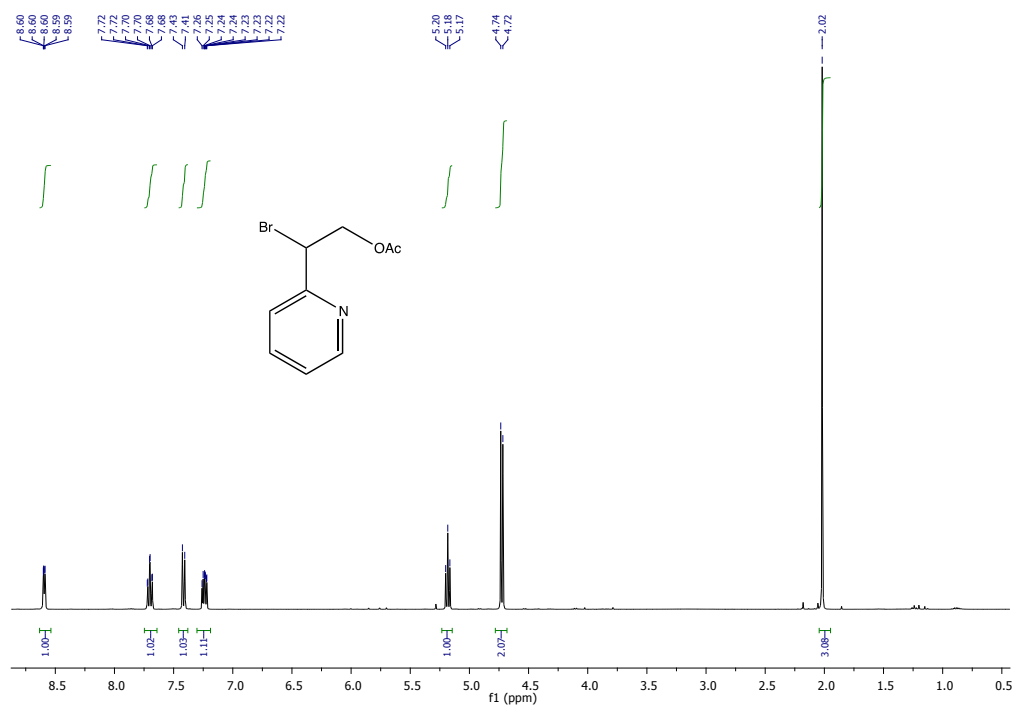
JP369\_D3AA\_CONE20\_MEX1\_copy 10 (0.188) AM2 (Ar,18000.0,0.00,0.00); Cm (1:10)

TOF MS ES+  
1.16e6

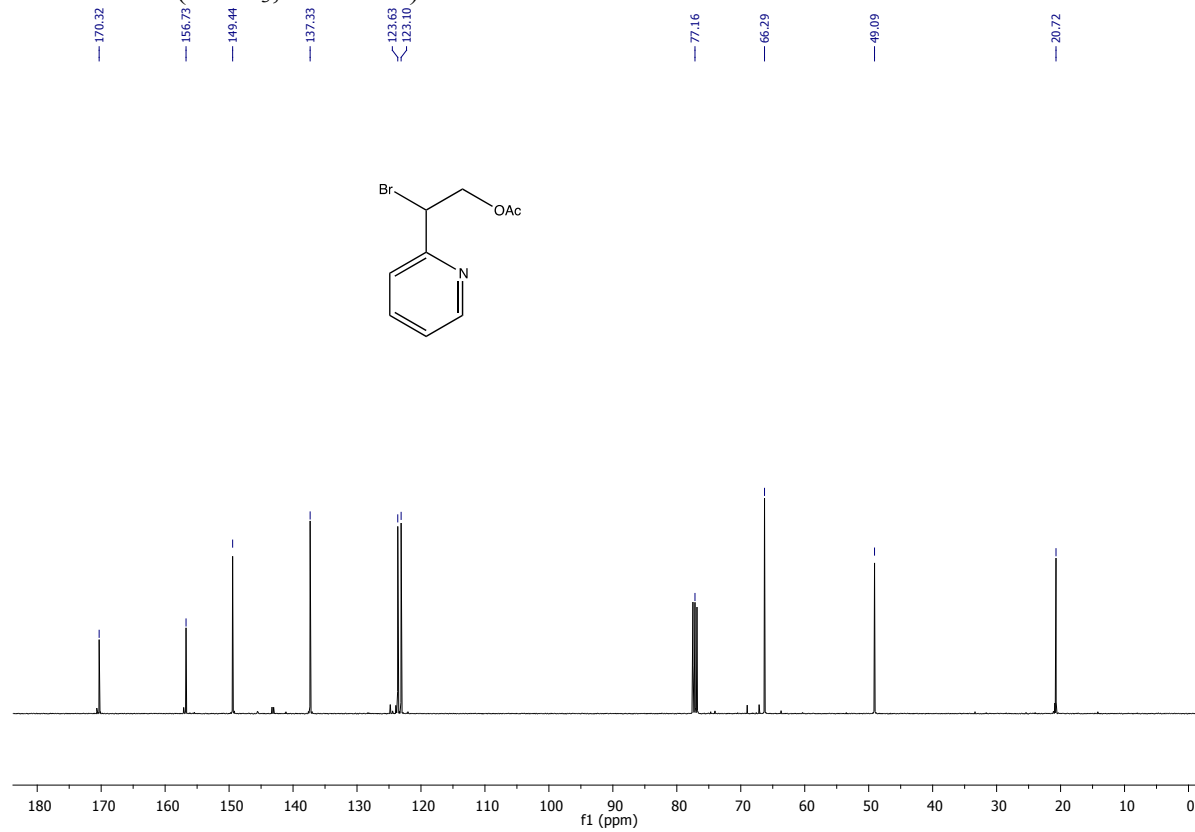


2-bromo-2-(pyridin-2-yl)ethyl acetate (**6b**).

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):



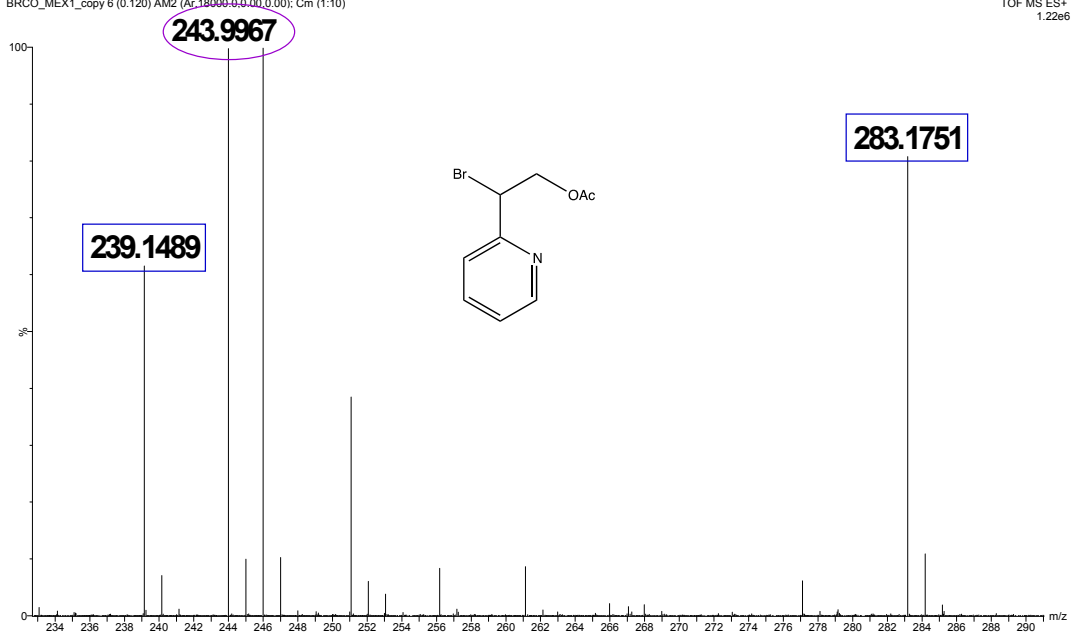
**6b**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz):



# 6b HRMS

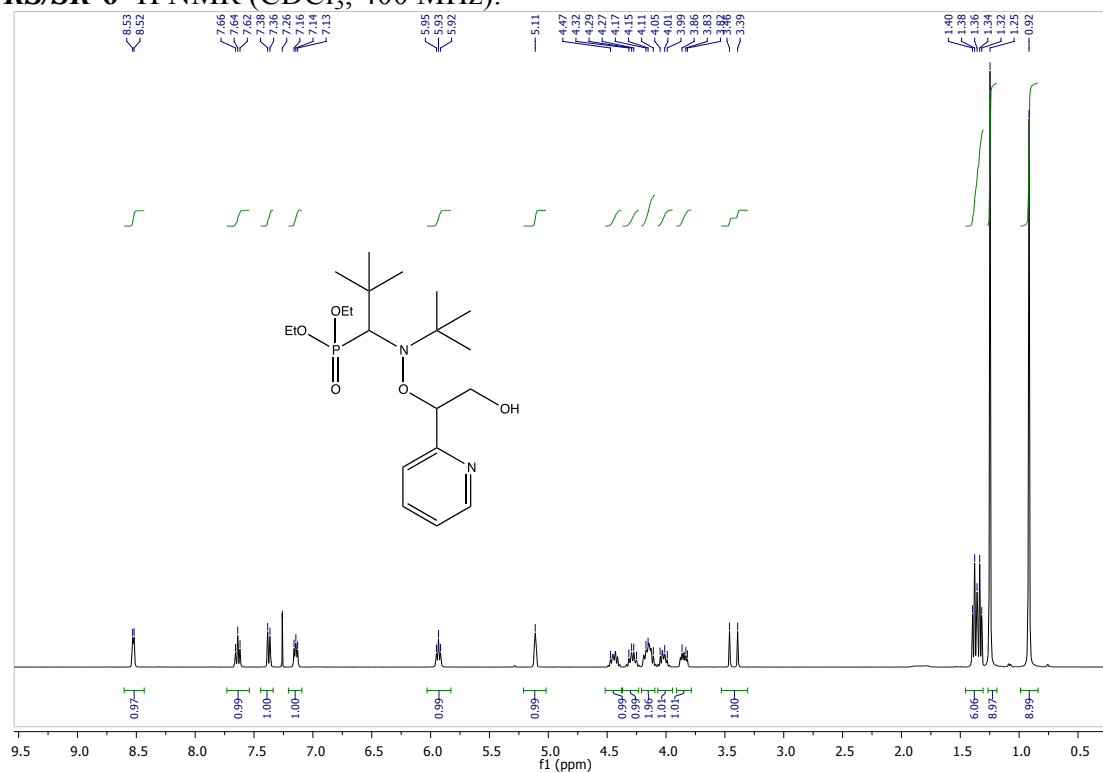
BRCO\_MEX1\_copy 6 (0.120) AM2 (Ar.18000-0.0.00.0.00): Cm (1:10)

TOF MS ES+  
1.22e6

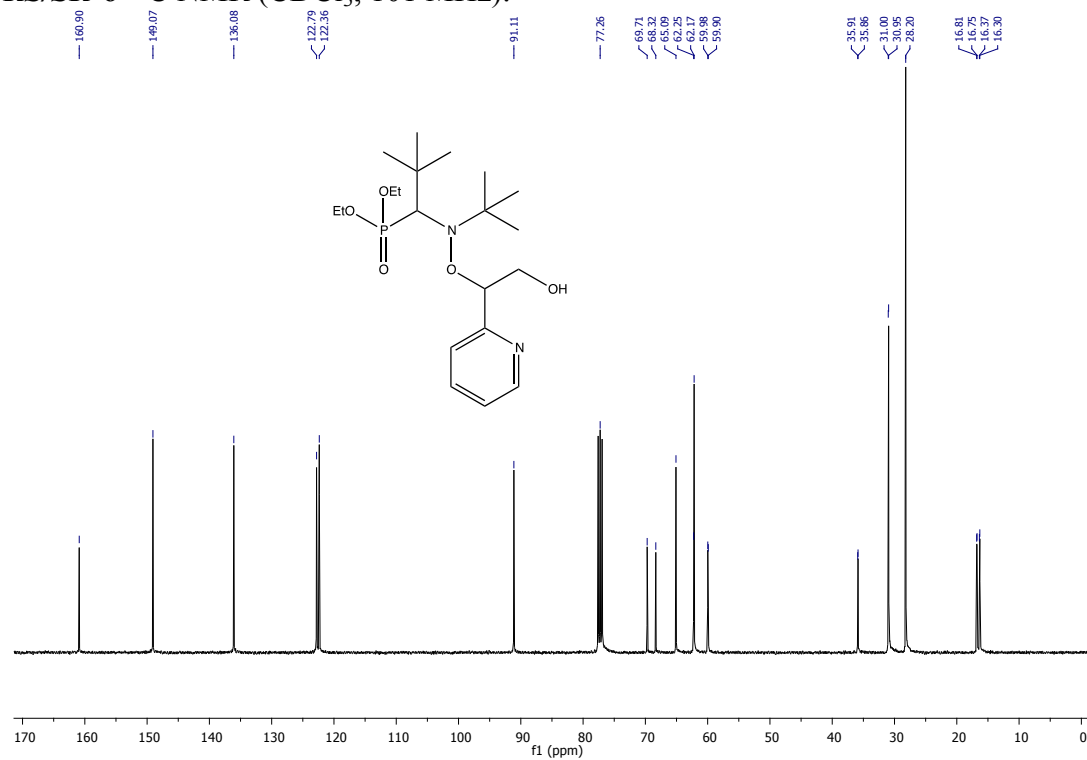


*Diethyl-(1-(tert-butyl-(2-hydroxy-1-(pyridin-2-yl)ethoxy)amino)-2,2-dimethylpropyl) phosphonate (6).*

**RS/SR-6**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):



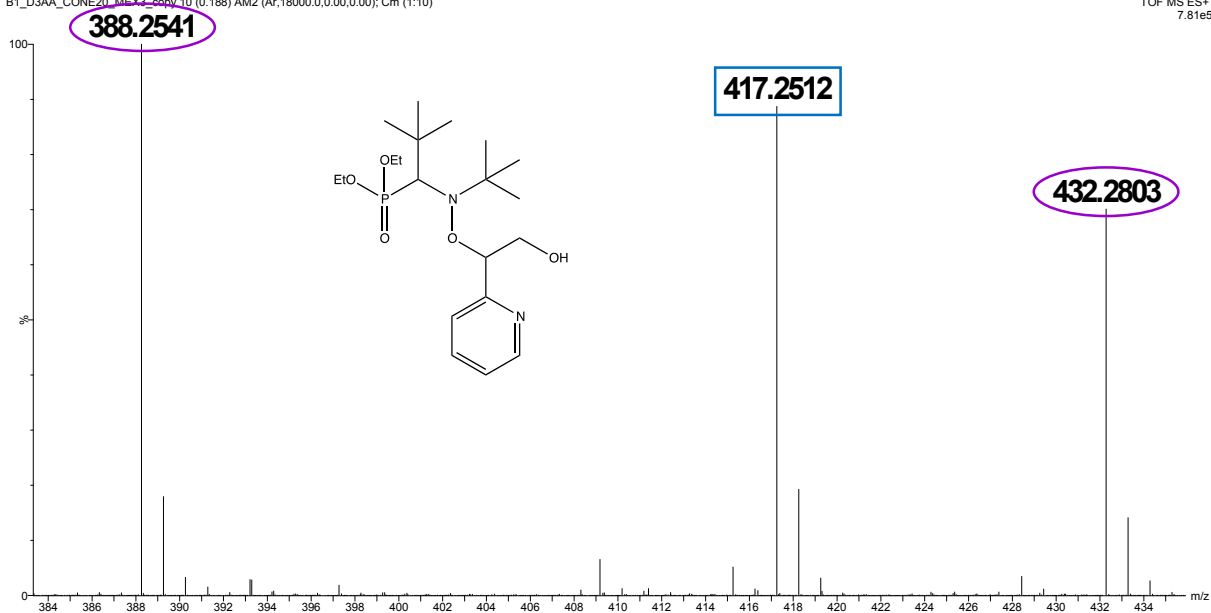
**RS/SR-6**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz):



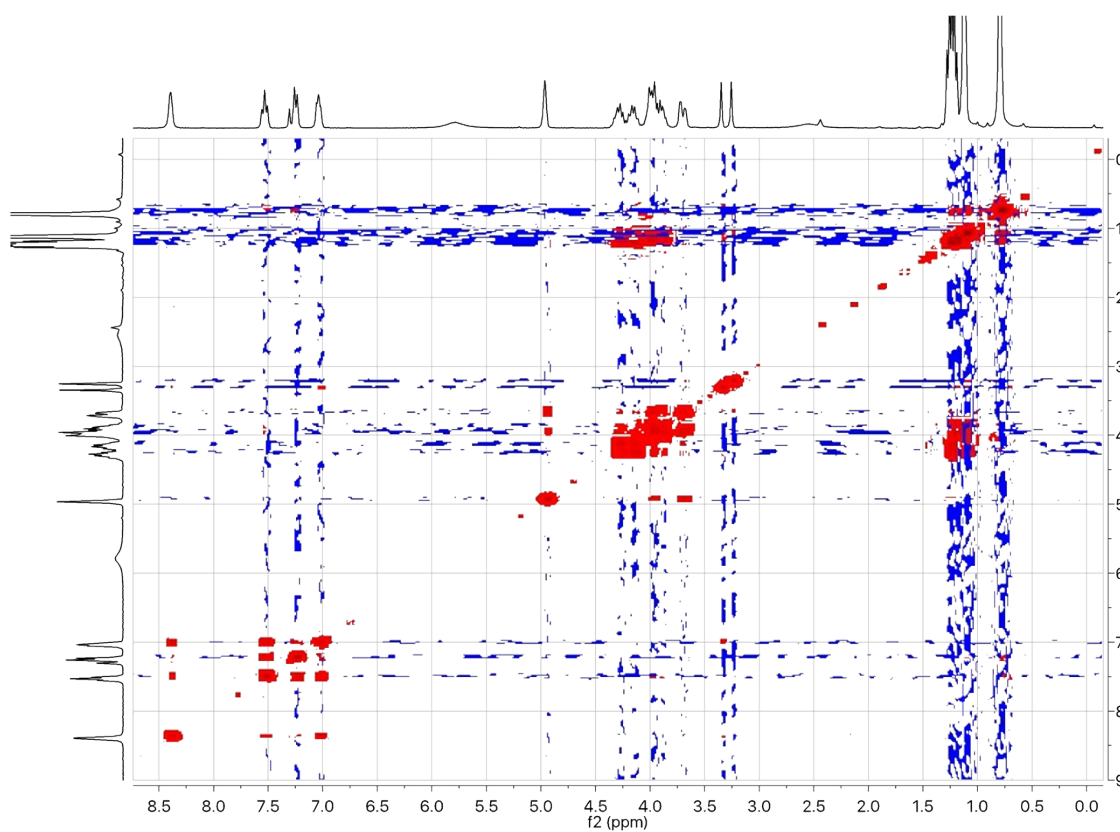
# RS/SR-6 HRMS

B1\_D3AA\_CONE20\_MEX2\_copy\_10 (0.188) AM2 (Ar,18000.0,0.00,0.00); Cm (1:10)

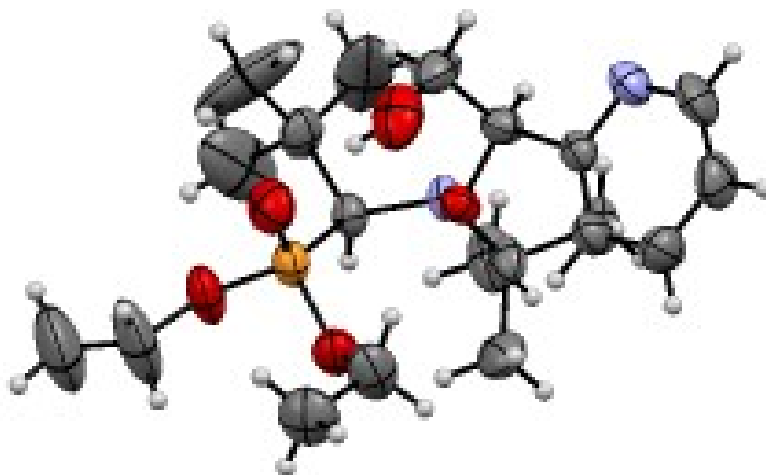
TOF MS ES+  
7.81e5



# RS/SR-6 COSY



*RS/SR-6* : The ellipsoid contour percent is given at 50% for the ORTEP plot.

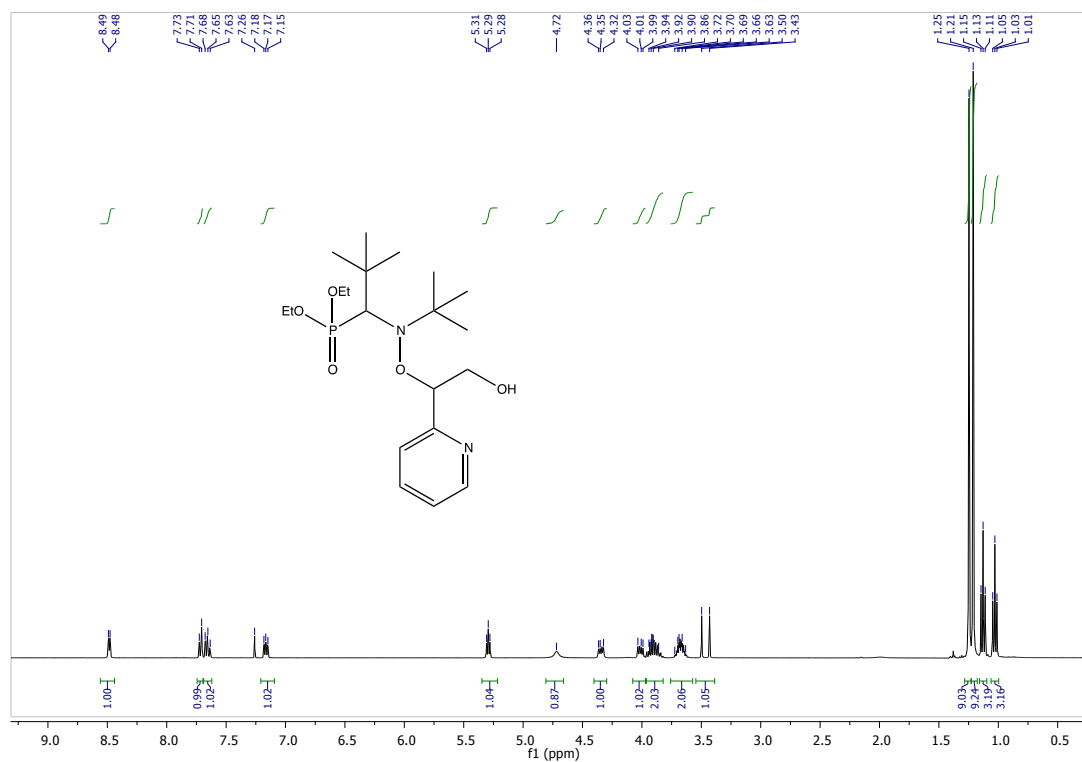


**Table 2SI.** XRD data for *RS/SR-6*

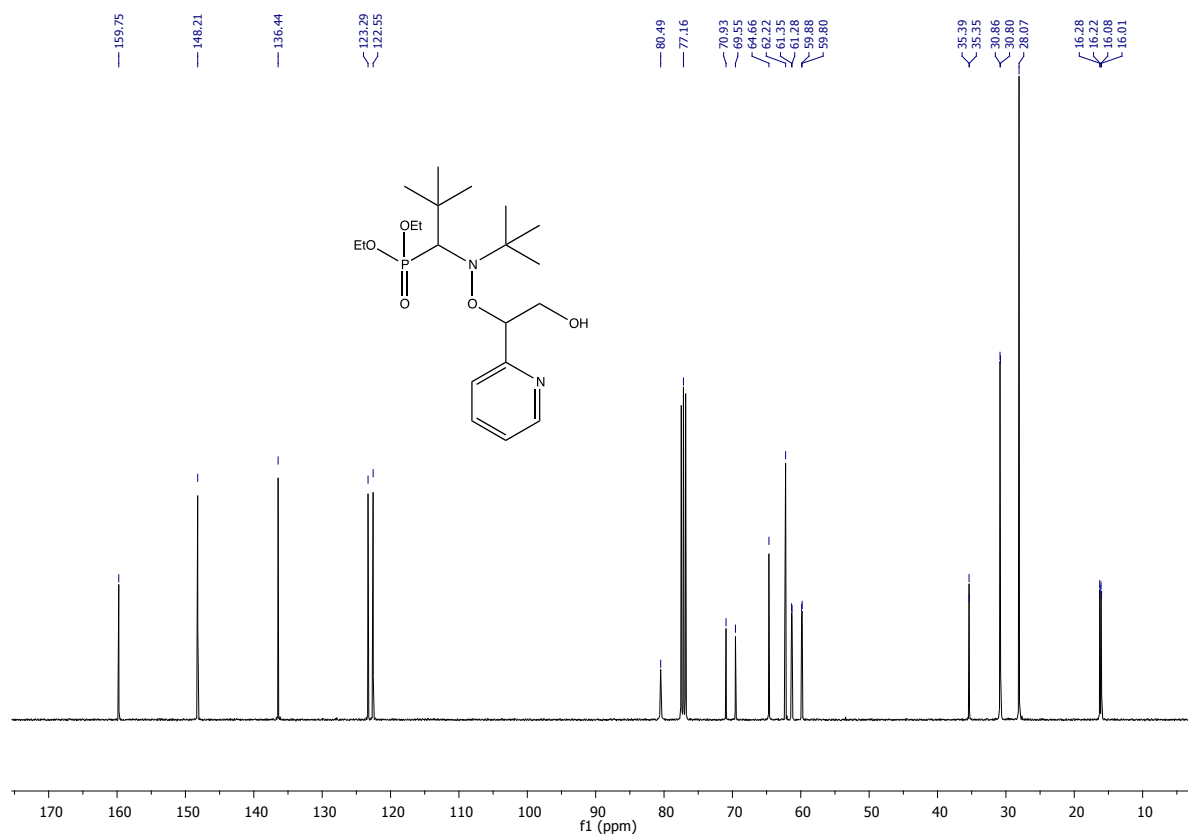
Empirical formula	C <sub>20</sub> H <sub>37</sub> N <sub>2</sub> O <sub>5</sub> P	$\mu/\text{mm}^{-1}$	0.148
Formula weight	416.48	F(000)	904.0
Temperature/K	293	Crystal size/mm <sup>3</sup>	0.26 × 0.18 × 0.08
Crystal system	monoclinic	Radiation	MoK $\alpha$ ( $\lambda = 0.71073$ )
Space group	P2 <sub>1</sub> /c	2 $\Theta$ range for data collection/ $^{\circ}$	7.064 to 55.41
a/ $\text{\AA}$	13.3358(4)	Index ranges	-16 ≤ h ≤ 16, -11 ≤ k ≤ 11, -25 ≤ l ≤ 24
b/ $\text{\AA}$	8.9190(3)	Reflections collected	15918
c/ $\text{\AA}$	19.7702(8)	Independent reflections	4783 [R <sub>int</sub> = 0.0272, R <sub>sigma</sub> = 0.0307]
$\alpha/^{\circ}$	90	Data/restraints/parameters	4783/0/262
$\beta/^{\circ}$	95.598(3)	Goodness-of-fit on F <sup>2</sup>	1.052
$\gamma/^{\circ}$	90	Final R indexes [I ≥ 2 $\sigma$ (I)]	R <sub>1</sub> = 0.0621, wR <sub>2</sub> = 0.1501
Volume/ $\text{\AA}^3$	2340.28(14)	Final R indexes [all data]	R <sub>1</sub> = 0.0852, wR <sub>2</sub> = 0.1665
Z	4	Largest diff. peak/hole / e $\text{\AA}^{-3}$	0.61/-0.48
$\rho_{\text{calc}}/\text{g}/\text{cm}^3$	1.182		



**RR/SS-6**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):



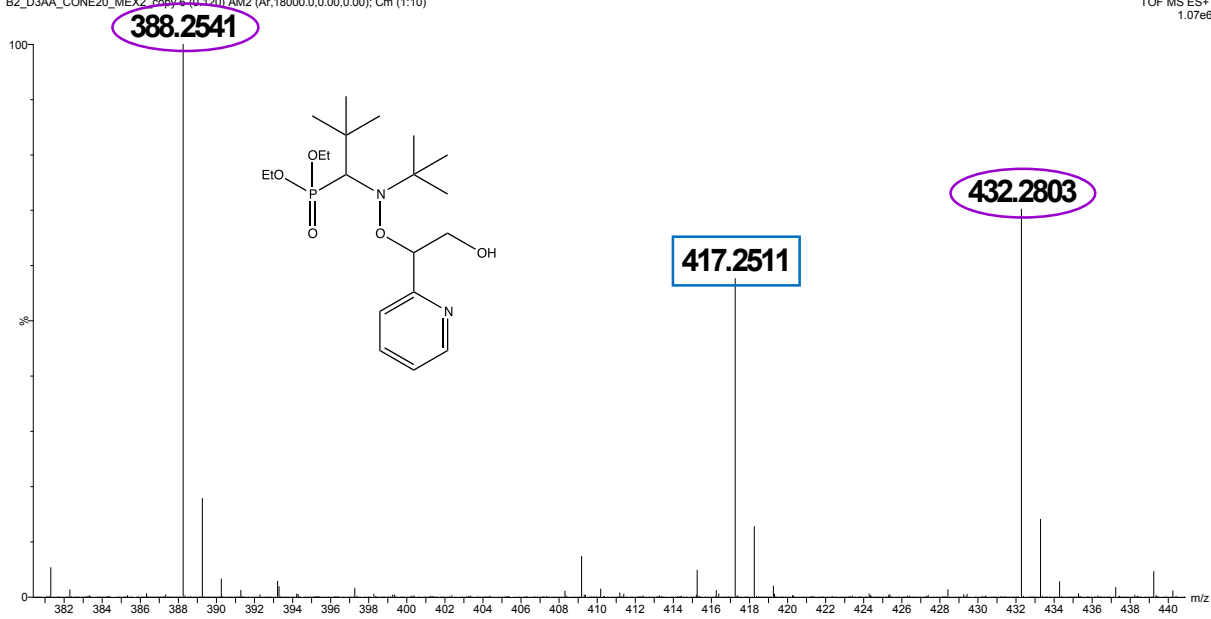
**RR/SS-6**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz):



# RR/SS-6 HRMS

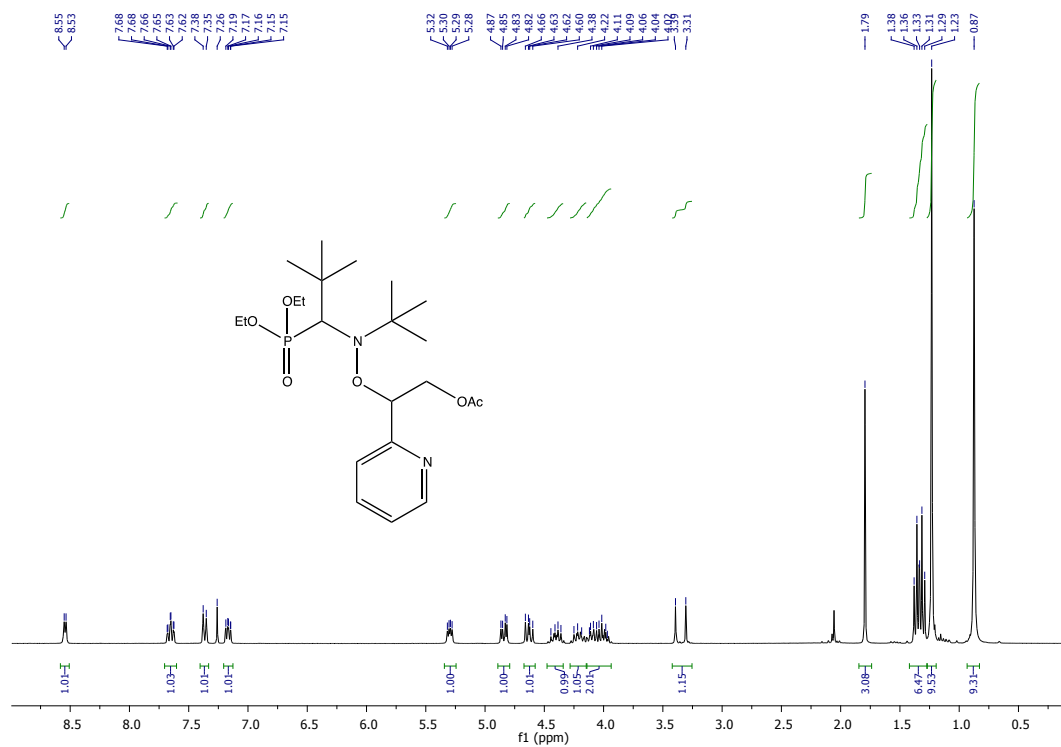
B2\_D3AA\_CONE20\_MEX2\_copy6 (6.120) AM2 (Ar, 18000.0, 0.00, 0.00); Cm (1:10)

TOF MS ES+  
1.07e6

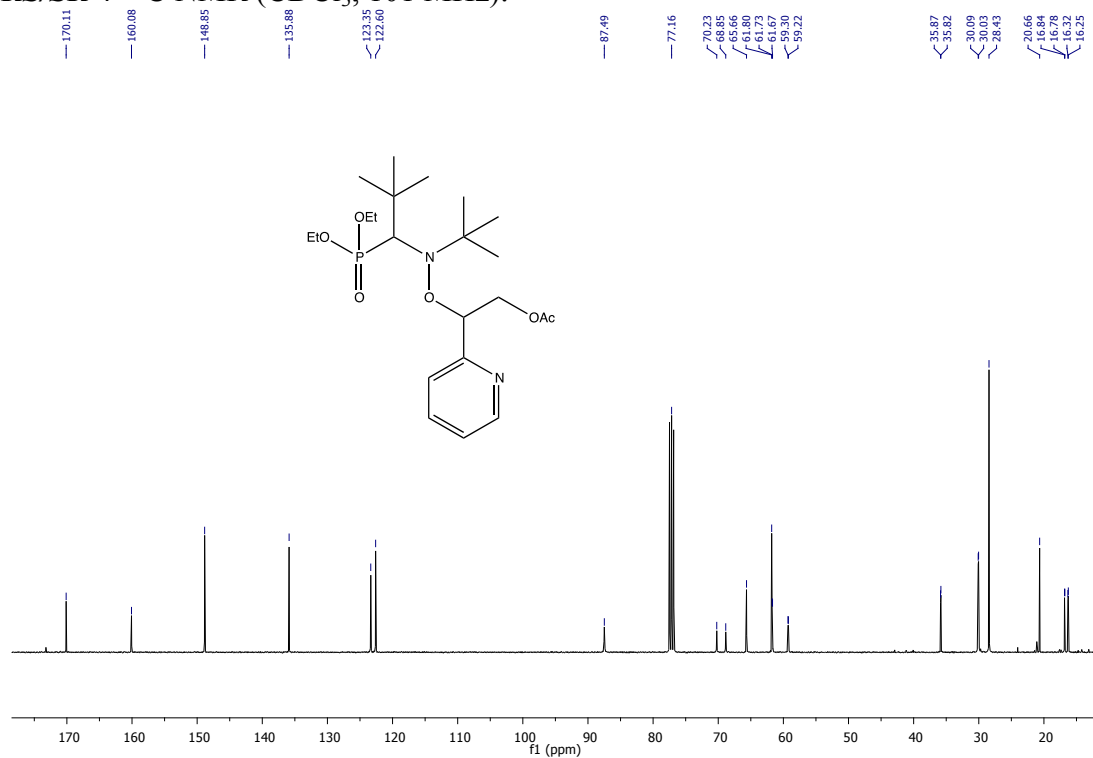


*(S)*-2-((*tert*-butyl((*R*)-1-(diethoxyphosphoryl)-2,2-dimethylpropyl)amino)oxy)-2-(pyridin-2-yl)ethyl acetate (**RS/SR-7**).

**RS/SR-7**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):



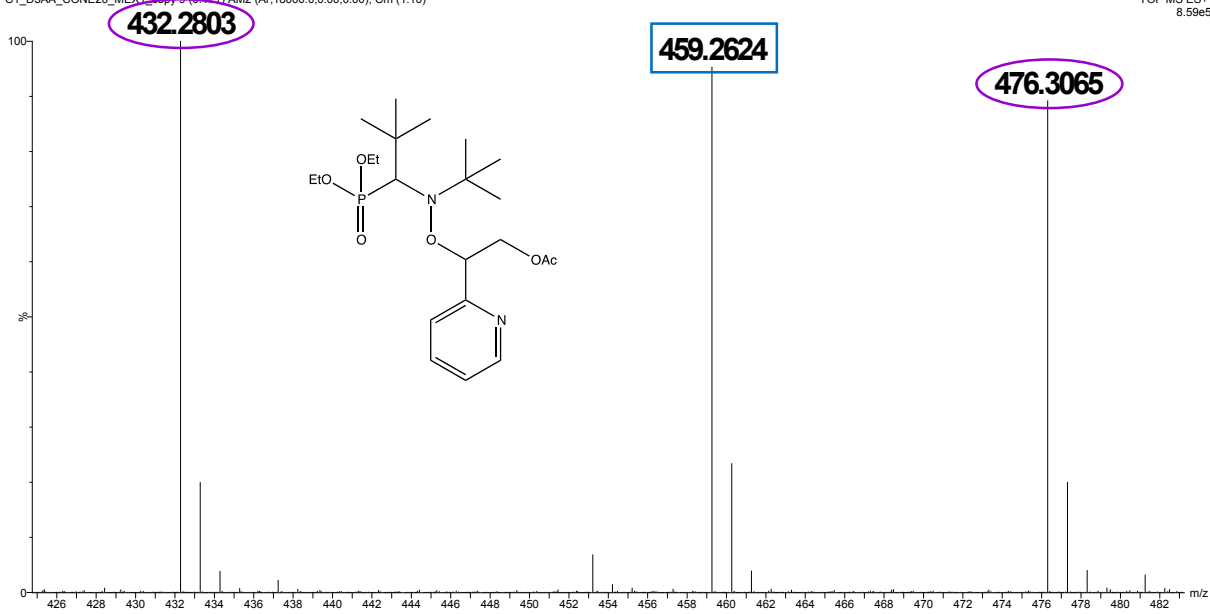
**RS/SR-7**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz):



# RS/SR-7 HRMS

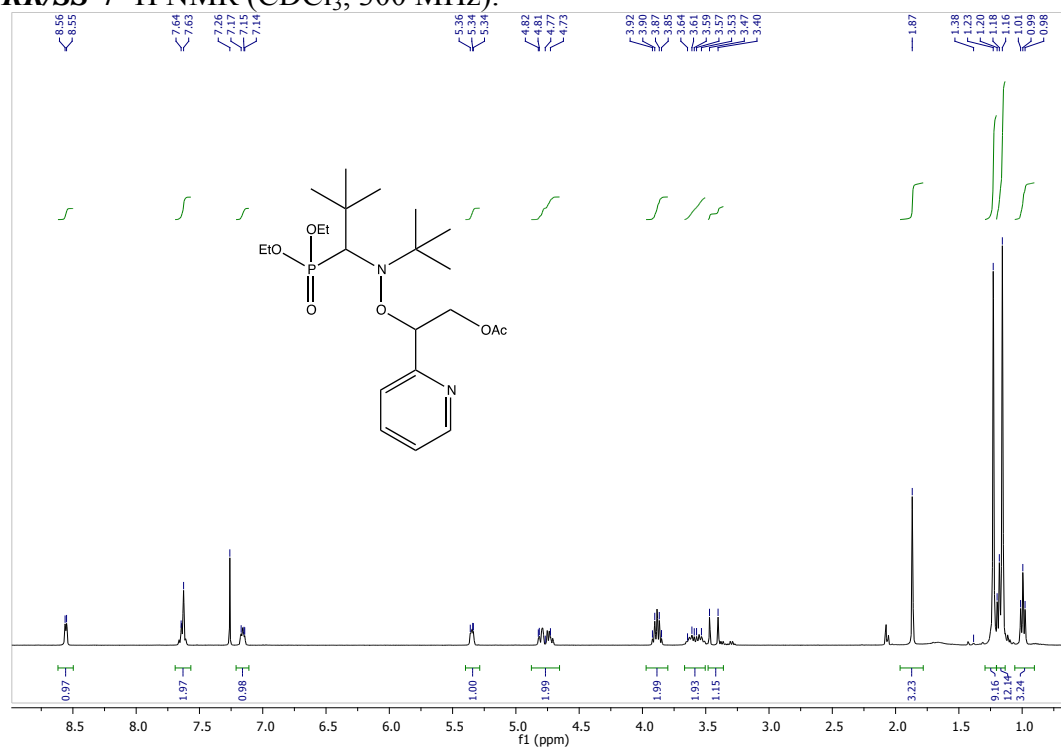
C1\_D3AA\_CONE20\_MEX1\_2019-06-17(1).AM2 (Ar,18000.0,0.00,0.00); Cm (1:10)

TOF MS ES+  
8.59e5

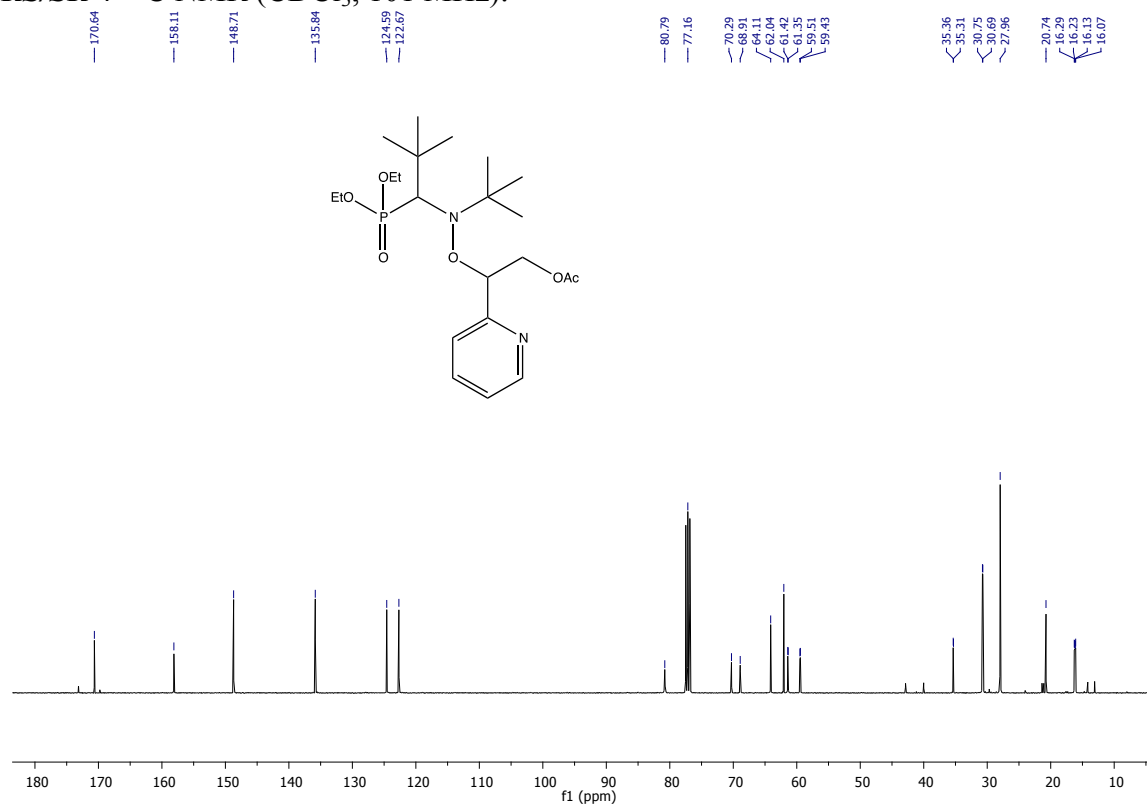


(*R*)-2-((*tert*-butyl((*R*)-1-(diethoxyphosphoryl)-2,2-dimethylpropyl)amino)oxy)-2-(pyridin-2-yl)ethyl acetate (**RR/SS-7**).

**RR/SS-7**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):



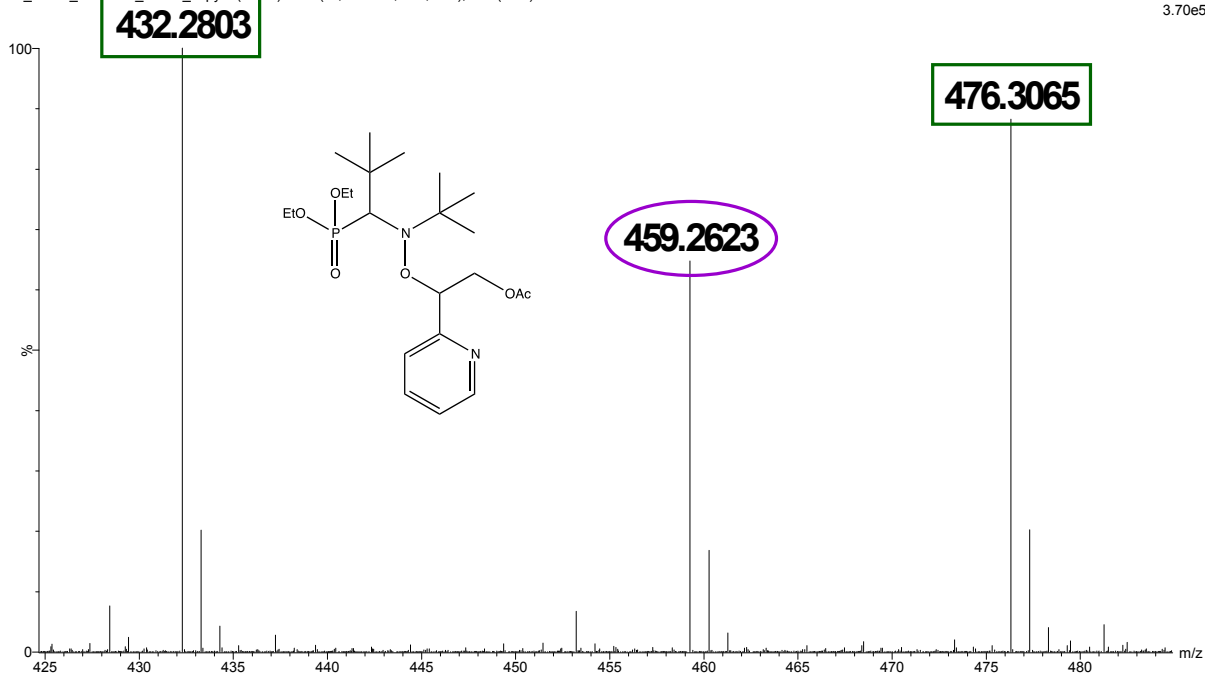
**RS/SR-7**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz):

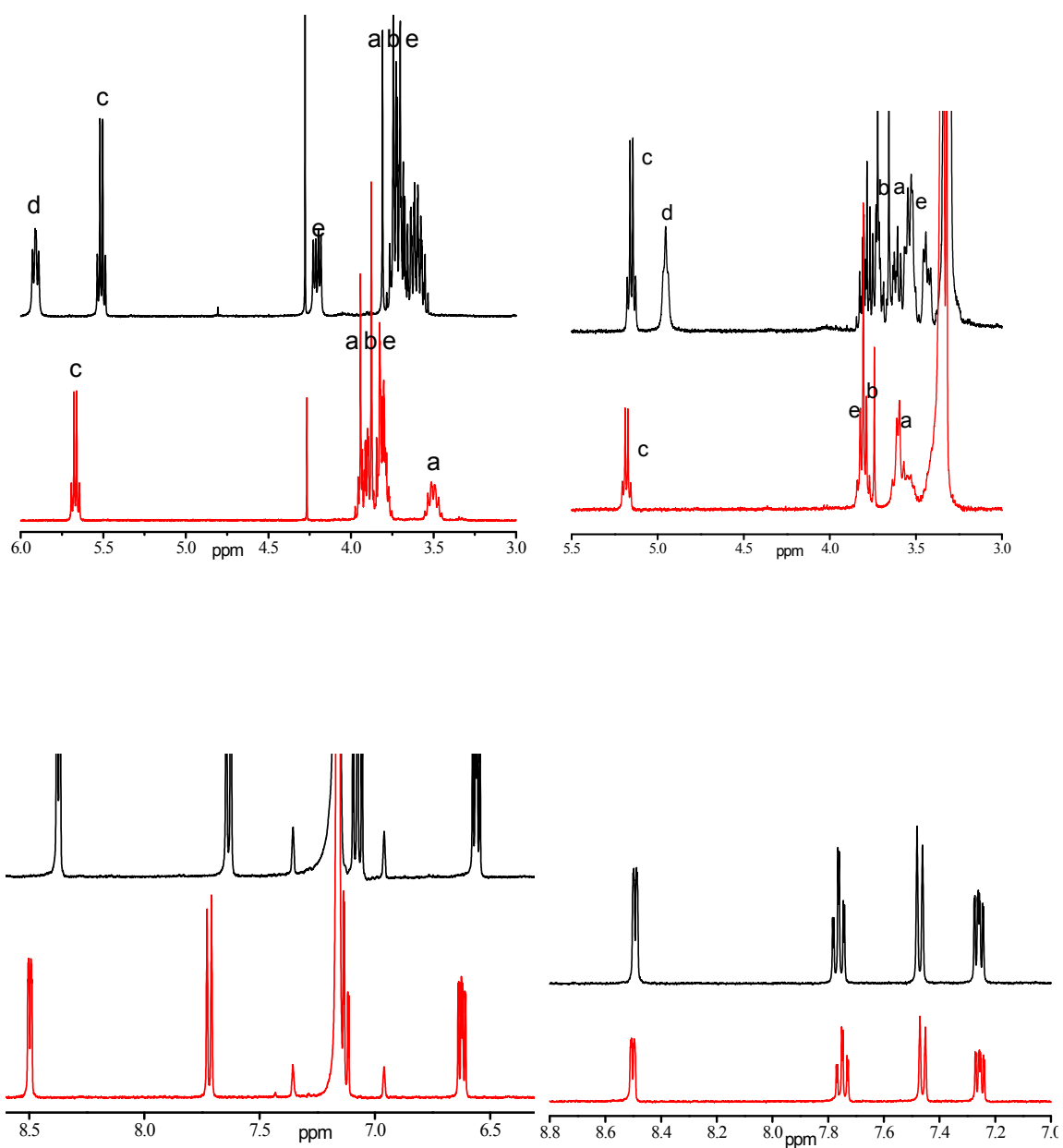


**RR/SS-7 HRMS**

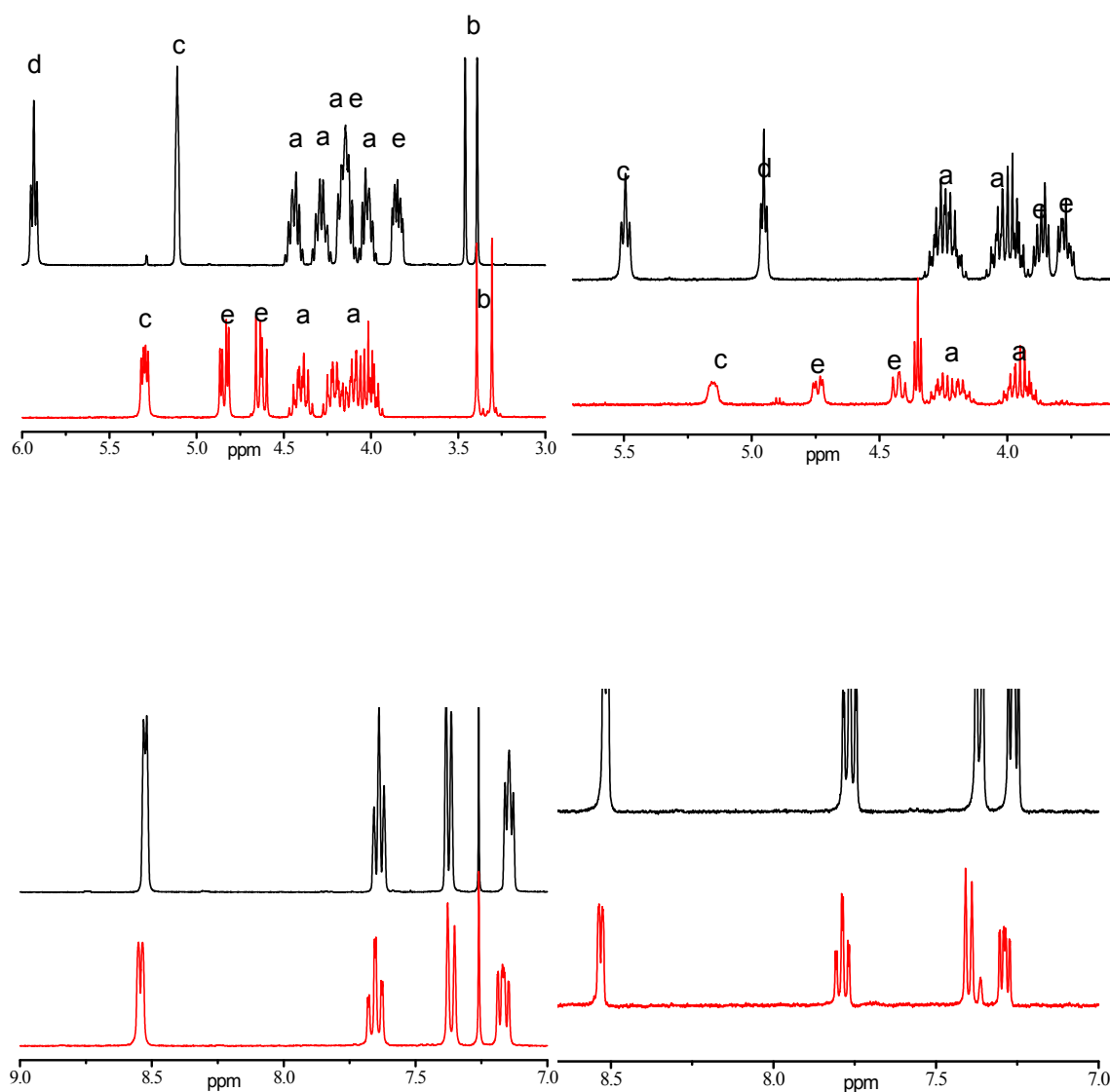
C2\_D3AA\_CONE20\_MEX3\_copy 1 (0.934) AM2 (Ar,18000.0,0.00,0.00); Cm (1:10)

TOF MS ES+  
3.70e5



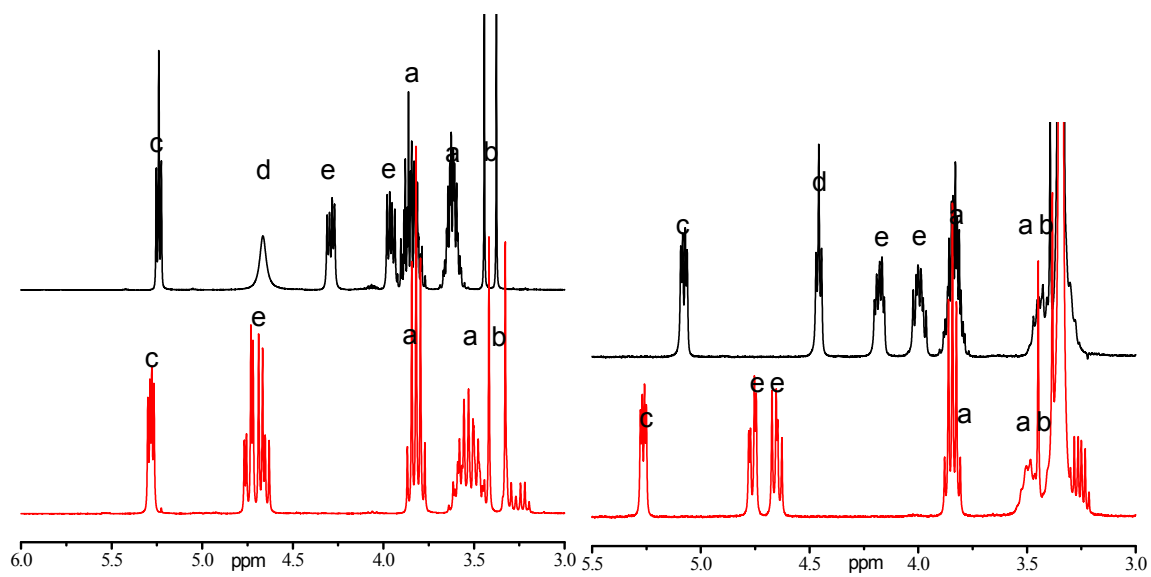


**Figure 1SI.**  $^1\text{H}$  NMR of *RS/SR-4* (top) and *RS/SR-5* (bottom) in the range 3 – 6 ppm (top row) and 6 – 9 ppm (aromatic proton zone, bottom row) in benzene- $d_6$  (left) and DMSO- $d_6$  (right). Labelling of protons  $\text{MeCH}_2\text{O}$ ,  $\text{CHP}$ ,  $\text{CHMe}$ ,  $\text{OH}$ , and  $\text{CH}_2\text{O}$  is a – e, respectively.

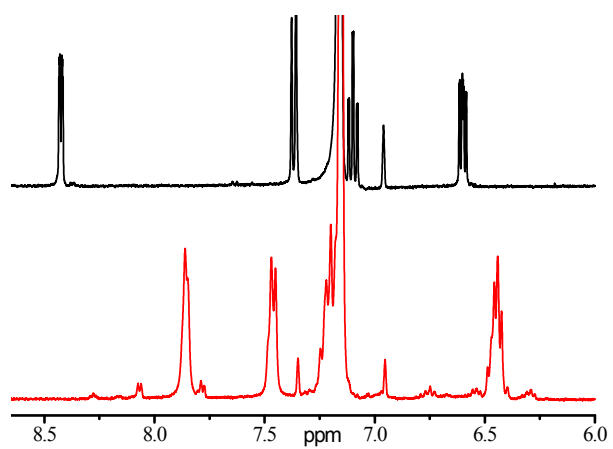


**Figure 2SI.**  $^1\text{H}$  NMR of *RS/SR-6* (top) and *RS/SR-7* (bottom) in the range 3 – 6 ppm (top row) and 6 – 9 ppm (pyridyl proton zone, bottom row) in  $\text{CDCl}_3$  (left) and  $\text{DMSO-}d_6$  (right). Labelling of protons  $\text{MeCH}_2\text{O}$ ,  $\text{CHP}$ ,  $\text{CHMe}$ ,  $\text{OH}$ , and  $\text{CH}_2\text{O}$  is a – e, respectively.

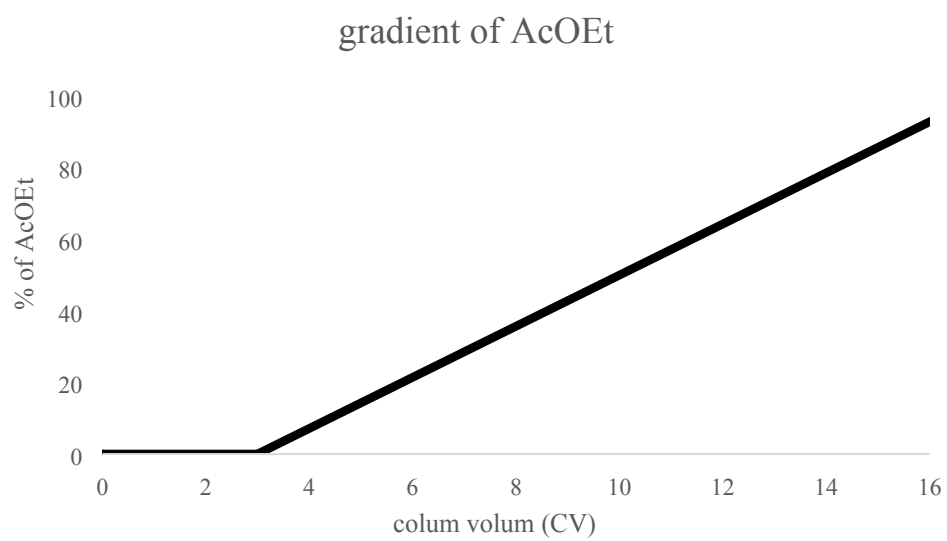




**Figure 3SI.**  $^1\text{H}$  NMR of *RR/SS-6* (top) and *RR/SS-7* (bottom) in the range 3 – 6 ppm in  $\text{CDCl}_3$  (left) and  $\text{DMSO}-d_6$  (right). Labelling of protons  $\text{MeCH}_2\text{O}$ ,  $\text{CHP}$ ,  $\text{CHMe}$ ,  $\text{OH}$ , and  $\text{CH}_2\text{O}$  is a – e, respectively.



**Figure 4SI.**  $^1\text{H}$  NMR of the aromatic zone for *RR/SS-4* in  $\text{C}_6\text{D}_6$  (top) and  $\text{C}_6\text{D}_6 + 1$  eq. TFA (bottom).



**Figure 5SI.** Gradient profile for the purification using Reveleris® machine.

**Free motions in the nitroxyl fragment.** The conformations of the nitroxide are controlled by *i*) the steric strain, *ii*) the hyperconjugation in the case of a strong electron acceptor bond such as the C—P bond of the diethylphosphoryl group carried by the nitroxide, and *iii*) the occurrence of IHB when the nitroxide carries H-donor groups such as a hydroxyl group and H-acceptor groups such as a diethylphosphoryl group. To address this issue, **2** and **3** were prepared via 3 routes (See Scheme 2): *i*) **3a**→**3b**→**3•**→**3**→**2**<sup>1</sup> with the protection of the hydroxyl group, which suppresses IHB in **3**, in the last step (**3**→**2**); *ii*) **3a**→**3b**→**2b**→**2•**→**2'**<sup>29</sup> with the protection of the hydroxyl group, which suppresses IHB, in the second step (**3b**→**2b**); *iii*) **3a**→**2a**→**2b**→**2•**→**2'**→**3'**<sup>29</sup> with the protection of the hydroxyl group in the starting materials **3a** suppressing the putative IHB which is regenerated in the last step (**2'**→**3'**).

### **Influence of IHB on $k_d$ .**

One must keep in mind that the suppression of the free hydroxyl group does not only suppress the effect of IHB, it also has an effect on the polarity and the steric strain, and the impact of each effect is different depending on its location on the alkyl or the nitroxyl fragment. Obviously, the bulkiness of SiMe<sub>2</sub>*t*-Bu, Me and MeCO is not the same and might induce very different strains, which might be enhanced or reduced depending on the configuration. Fortunately, it seems that in our models the steric effect due to the size of the protecting group can be disregarded (see articles on levelled steric effect and effect of the penultimate unit on  $k_d$ ). Moreover, the polar effect of electron withdrawing groups (EWG) also has an influence on  $k_d$ , thus the protecting groups are selected to afford either a weaker polar effect, as with CH<sub>2</sub>OSiMe<sub>2</sub>*t*-Bu ( $\sigma_1 = 0$ ), a stronger polar effect as with CH<sub>2</sub>OAc ( $\sigma_1 = 0.15$ ), or a similar polar effect, as with CH<sub>2</sub>OMe ( $\sigma_1 = 0.11$ ) compared with the OH group ( $\sigma_1 = 0.11$ ). However, this polar effect differs when it is applied on the alkyl of nitroxyl fragment. That is, a strong EWG carried by the nitroxyl affords, in general, a decrease in  $k_d$ , whereas when carried by the alkyl fragment it affords an increase in  $k_d$ .

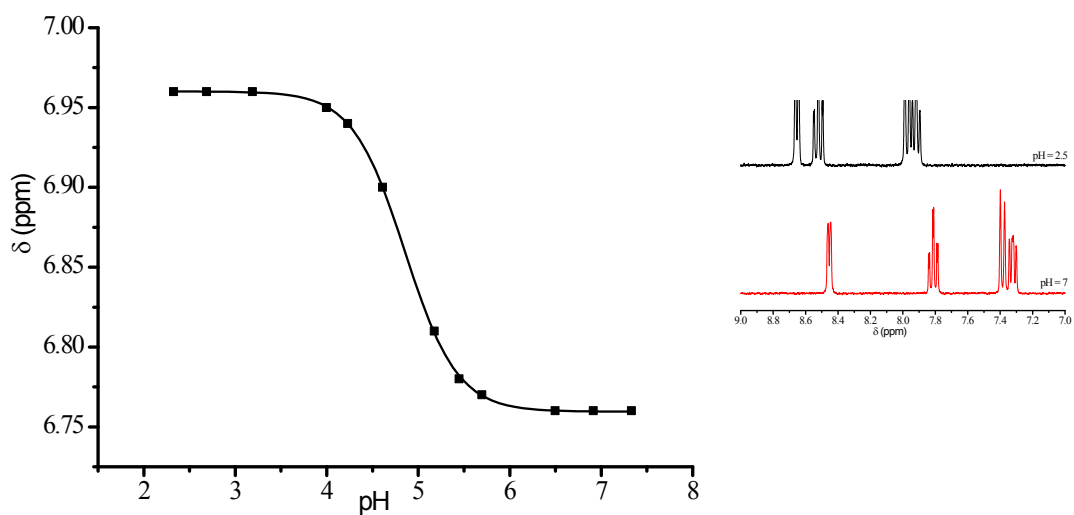
Several types of IHB are possible – *intraR* and *interR*, and *intraN* and *interN* (Figure 4) – and are observed in **4** and **6** depending on the diastereoisomer. NMR data, X-ray and DFT calculations show that *interR* IHB occurs for diastereoisomers *RS/SR* of **6** and **9**, that *intraR* IHB occurs for *RR/SS*-**6**, that *intraN* IHBs occur for **3** and *RS/SR*-**4**, and for *RR/SS*-**4** both *intraN* and *interN* IHBs are reported. Thus, to determine various increments, alkoxyamines **3** for *intraN* IHB, **9** for *interR* IHB, **2** and **10** for the protected hydroxyl group, and **12** for the pyridyl moiety (see Table 4) were selected as reference models. As changes in  $E_a$  between diastereoisomers are due to small structural changes and as there is no reason for them to be the same for each diastereoisomer,  $E_a'$  values are estimated for each diastereoisomer to afford a range in which experimental data are expected to be observed. As seen in Table 4, differences between the closest  $E_a'$  values and the experimental  $E_a$  values are in the range 0.9 – 2.7 kJ/mol,<sup>2</sup> meaning that the group additivity approach still holds and provides rather accurate values.

**IHB in alkoxyamines.** The *interR* IHB in *RS/SR-6* observed by X-ray and NMR is nicely confirmed by DFT calculations. Conformer **A** is more stable than conformers **B** and **C** by 5 and 19 kJ/mol, respectively. Changes in NMR signals for diastereoisomer *RR/SS-6* are ascribed to *intraR* IHB, which is nicely supported by DFT calculations showing that conformer **B** is more stable than conformers **A** and **C** by 10 and 17 kJ/mol, respectively. Moreover, DFT calculations show that conformer **B** of *RR/SS-6* is less stable than conformer **A** of *RS/SR-6* by 14 kJ/mol, in good agreement with the 6.5 kJ/mol lower  $E_a$ . Changes in NMR signals for *RS/SR-4* (similar to those of **3**)<sup>3</sup> are ascribed to *intraN* IHB and supported by DFT calculations showing that conformer **A** is more stable than conformers **B** and **C** by 6.1 and 22.1 kJ/mol, respectively.

### **p*K*<sub>a</sub> measurement for 2-hydroxyethylpyridine.**

p*K*<sub>a</sub> values of 2-hydroxyethylpyridine was measured by monitoring the dependency of <sup>1</sup>H NMR chemical shift in various pH\*. A solution of 0.01 M 2-hydroxyethylpyridine in D<sub>2</sub>O/CD<sub>3</sub>OD (1/1) was used. The pH\* values were adjusted with DCl and NaOD and converted to pH values with the equation  $\text{pH} = 0.929 \text{ pH}^* + 0.42$ . <sup>1</sup>H-NMR spectra were recorded on 400 MHz spectrometer.

This procedure was applied to determine p*K*<sub>a</sub> values stored in Table 3.

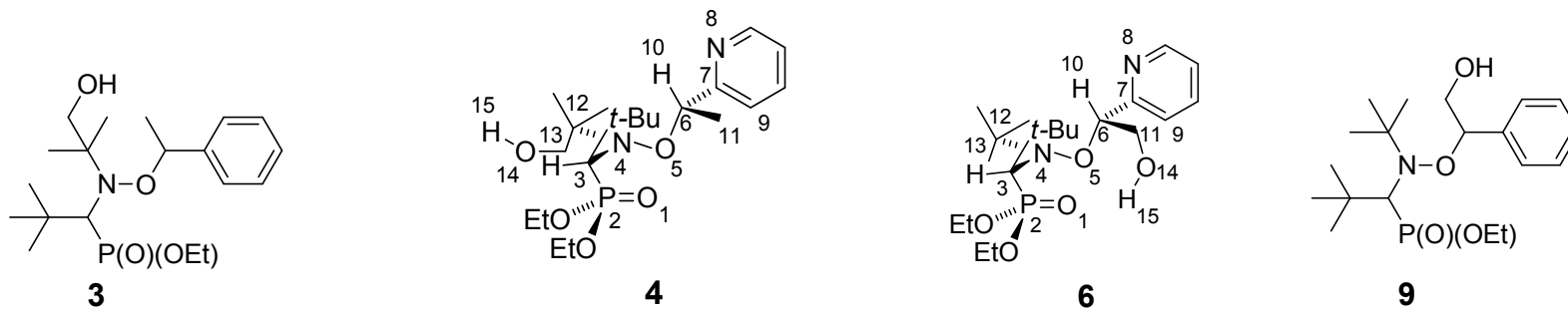


## **DFT calculation**

All calculations were performed using Gaussian package 09, revision A02.<sup>4</sup>

The geometry of the species were optimized at the M062X/6-31+G(d,p) level of theory. Vibrational frequencies were calculated at M062X/6-31+G(d,p) level to insure that the obtained geometries are minima (no imaginary frequency). The vibrational frequencies were scaled by a usual factor of 0.967. The corresponding thermal corrections were included to obtain the enthalpy and Gibbs free energy values under the standard conditions ( $p = 1$  atm and  $T = 298.15$  K). Values are given in u.a.



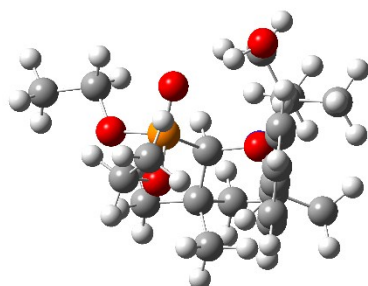


**Table 3SI.** Geometrical parameters for conformations **A**, **B**, and **C** of **3**, **4**, **6**, and **9**

	RR/SS- 3 <i>Conf A</i>	RS/SR- 3 <i>Conf A</i>	RR/SS- 4 <i>Conf A</i>	RR/SS- 4 <i>Conf B</i>	RR/SS- 4 <i>Conf C</i>	RS/SR- 4 <i>Conf A</i>	RS/SR- 4 <i>Conf B</i>	RS/SR- 4 <i>Conf C</i>	RR/SS- 6 <i>Conf A</i>	RR/SS- 6 <i>Conf B</i>	RR/SS- 6 <i>Conf C</i>	RS/SR- 6 <i>Conf A</i>	RS/SR- 6 <i>Conf B</i>	RS/SR- 6 <i>Conf C</i>	RR/SS- 9 <i>Conf C</i>	RS/SR- 9 <i>Conf A</i>	RS/SR- 4 RX	RR/SS- 6 RX
bond length $l(\text{\AA})$																		
O5–C6	1.435	1.430	1.433	1.439	1.439	1.430	1.435	1.435	1.448	1.423	1.425	1.431	1.430	1.443	1.432	1.442	1.447	1.450
N4–O5	1.426	1.422	1.426	1.431	1.429	1.425	1.424	1.426	1.431	1.427	1.435	1.434	1.431	1.440	1.435	1.435	1.460	1.462
C3–P2	1.849	1.855	1.845	1.850	1.851	1.851	1.850	1.850	1.858	1.849	1.857	1.853	1.859	1.861	1.854	1.849	1.835	1.837
P2–O1	1.491	1.489	1.492	1.486	1.485	1.493	1.487	1.484	1.493	1.485	1.484	1.492	1.487	1.486	1.486	1.492	1.468	1.467
distance $d(\text{\AA})$																		
N4----C6	2.418	2.411	2.416	2.394	2.400	2.406	2.426	2.410	2.490	2.396	2.411	2.427	2.392	2.462	2.406	2.426	2.405	2.427
O1----C7	4.886	4.279	4.820	5.147	5.180	4.080	3.520	4.509	5.215	4.064	3.854	5.177	4.752	4.078	3.607	5.278	4.773	5.200
valence angle $\alpha(^{\circ})$																		
<N4O5C6>	115.34	115.38	115.34	113.03	113.61	115.04	116.07	114.73	119.75	114.21	114.91	115.78	113.52	117.32	114.14	115.03	111.66	112.88
<C3N4O5>	107.19	107.86	106.75	107.90	107.96	108.64	108.52	109.30	106.13	105.56	108.24	106.04	107.73	105.36	108.56	107.07	107.69	107.32
torsion angle $\theta(^{\circ})$																		
<O5C6C7C9>	-142.45	158.16	-35.37	-58.52	-41.82	-9.79	-125.83	28.21	-63.15	-14.74	132.67	-135.59	-94.56	49.38	-60.26	51.77	-13.64	-47.39

<C6O5N4nσ,N4> <sup>a</sup>	2.66	-17.88	4.59	-1.82	-0.07	21.72	12.82	17.98	11.19	19.27	9.11	6.15	-16.04	21.89	-21.7	2.51	-5.56	4.2
<O1P2C3N4>	94.08	48.49	-42.85	87.00	87.56	-49.32	76.79	84.56	-87.90	-81.30	-95.06	-86.61	-78.85	-89.72	-81.15	-86.39	73.19	85.85
<C7C6O5N4>	114.81	174.73	-116.87	-112.07	-113.47	173.51	-177.46	-167.99	26.69	-113.26	-93.15	104.99	66.83	-165.36	-179.46	101.88		134.84
<b>Δ G(kJ/mol)</b>	<b>88.09</b>	<b>94.92</b>	<b>85.67</b>	<b>-</b>	<b>-</b>	<b>91.44</b>	<b>-</b>	<b>-</b>	<b>-</b>	<b>86.60</b>	<b>-</b>	<b>100.41</b>	<b>-</b>	<b>-</b>	<b>89.83</b>	<b>107.63</b>	<b>-</b>	<b>-</b>
<sup>a</sup> <nNOC>	=					<C <sub>6</sub> O <sub>5</sub> N <sub>4</sub> C <sub>3</sub> >					-							

RS/SR-3 Conf A

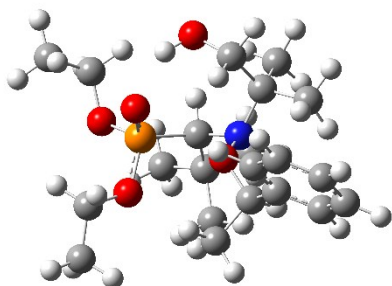


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#### RR/SS-3 Conf A

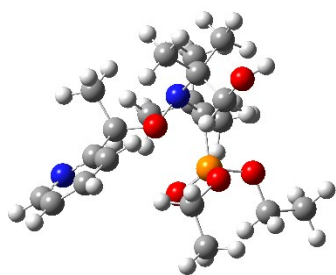


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**RS/SR- 4- Conf C**

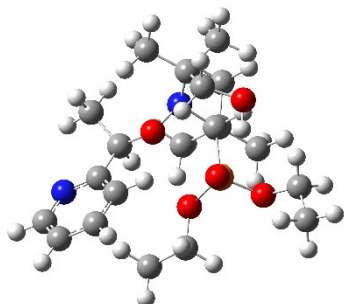


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C	-1.347876	-3.295304	1.281484
H	-2.343655	-2.841130	1.299179
H	-1.243785	-3.907419	2.181680
H	-1.286120	-3.963182	0.420322
C	1.106455	-3.042403	1.356817
H	1.190643	-3.750524	0.527300
H	1.129333	-3.590274	2.301302
H	1.965690	-2.369643	1.332324
C	-0.337515	-1.326670	2.476286
H	0.494094	-0.618292	2.471234
H	-1.264770	-0.743102	2.420642
C	-1.460295	-0.771401	-0.357731
H	-2.239145	-1.050967	0.362279
C	-2.037672	-1.137450	-1.774757
C	-2.338951	-2.641359	-1.795773
H	-1.427035	-3.222514	-1.632693
H	-2.745760	-2.915113	-2.774875
H	-3.077389	-2.919698	-1.035237
C	-1.070792	-0.835246	-2.925469
H	-0.782228	0.218306	-2.949277
H	-1.567194	-1.078550	-3.871494
H	-0.175571	-1.457629	-2.859727
C	-3.352550	-0.384426	-2.035692

H	-4.058277	-0.492473	-1.205252
H	-3.816350	-0.793872	-2.939040
H	-3.184033	0.683758	-2.201058
C	-3.241084	2.753183	0.339814
H	-2.820692	3.310361	-0.505119
H	-2.828704	3.159512	1.271016
C	-4.754267	2.801634	0.336577
H	-5.144930	2.385631	-0.595624
H	-5.097245	3.835763	0.428967
H	-5.157323	2.223813	1.172172
C	0.623951	2.094882	1.351338
H	1.181392	1.929847	0.426921
H	1.183188	1.656356	2.183499
C	0.354549	3.569922	1.569272
H	-0.177088	3.981234	0.706202
H	1.298703	4.111176	1.681984
H	-0.246712	3.724987	2.469727
C	2.133624	-1.993696	-1.614506
H	2.787613	-2.481939	-0.886723
H	1.258716	-2.624394	-1.783896
H	2.683727	-1.876243	-2.551954
H	1.222240	-0.051187	-1.932148

#### RS/SR- 4- Conf A



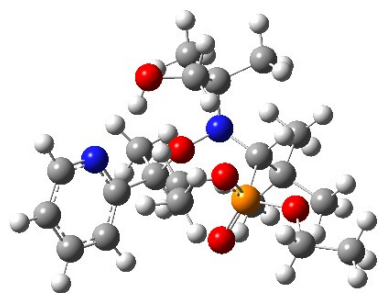
ZPE = 0.551488  
E = -1610.306542  
H = -1610.305598  
G = -1610.398935

P	0.766152	-1.210795	0.161619
O	-0.497670	1.156081	0.341184
O	2.280222	0.553127	2.523878
H	1.771604	-0.272729	2.483195
O	0.436272	-1.222074	1.618647
O	-0.442248	-1.539585	-0.828608
O	1.792502	-2.405557	-0.187472
N	0.809258	1.545153	-0.073123
N	-3.882960	0.871021	-0.745013
C	-1.518000	1.321443	-0.643657
C	-2.760783	0.696932	-0.037457
C	-2.715765	-0.057783	1.140143
H	-1.775752	-0.191521	1.666081
C	-3.892512	-0.651585	1.586926
H	-3.890641	-1.247738	2.494894

C	-5.063804	-0.477226	0.855736
H	-6.001768	-0.923400	1.168402
C	-5.001883	0.295256	-0.302376
H	-5.892301	0.459842	-0.905294
C	1.367283	2.336048	1.080911
C	2.805389	2.767246	0.792278
H	3.494383	1.924977	0.708726
H	3.149421	3.370965	1.637378
H	2.863344	3.379264	-0.110157
C	0.506274	3.594482	1.219331
H	0.466151	4.133170	0.268773
H	0.943054	4.256513	1.972632
H	-0.512238	3.347231	1.527231
C	1.323614	1.592670	2.427351
H	1.538722	2.328316	3.213573
H	0.312534	1.202704	2.587537
C	1.556242	0.329842	-0.492951
H	2.512287	0.307776	0.049319
C	1.936848	0.356808	-2.019243
C	0.736165	0.447946	-2.966920
H	0.047101	-0.391818	-2.847119
H	1.104248	0.440245	-3.998751
H	0.194874	1.387054	-2.819388
C	2.778969	-0.870303	-2.402681
H	3.595189	-1.036940	-1.689641
H	3.223726	-0.697943	-3.388164
H	2.184149	-1.784408	-2.451060
C	2.796988	1.606129	-2.258931
H	2.239458	2.512573	-2.010135
H	3.075834	1.654132	-3.316793
H	3.719144	1.584271	-1.668292
C	-1.278086	-2.684082	-0.537123
H	-1.569631	-2.641621	0.517543
H	-0.686095	-3.589237	-0.710415
C	-2.482996	-2.617072	-1.449252
H	-3.061900	-1.709524	-1.256649
H	-3.126607	-3.483485	-1.272606
H	-2.171993	-2.621101	-2.497305
C	2.810722	-2.769018	0.763939
H	3.114959	-1.889129	1.344093
H	3.664323	-3.091035	0.161344
C	2.316644	-3.878309	1.671087
H	1.466651	-3.527258	2.260808
H	3.115374	-4.192653	2.349329
H	2.007140	-4.741148	1.074912
C	-1.726389	2.762589	-1.077249
H	-2.058390	3.380291	-0.238393
H	-0.791277	3.166297	-1.473925
H	-2.493591	2.789829	-1.853202
H	-1.270009	0.707926	-1.516014

**RS/SR- 4- Conf B**



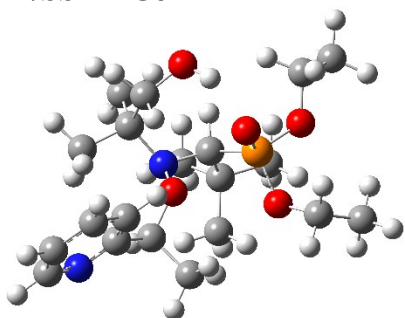


ZPE = 0.551438  
 E = -1610.302742  
 H = -1610.301798  
 G = -1610.396619

P	-1.189429	1.059338	-0.034476
O	0.743403	-0.786076	-0.040327
O	1.957999	-1.499126	2.336395
H	2.210528	-1.139991	1.469102
O	-0.570035	1.641510	-1.255047
O	-2.639412	1.649216	0.344284
O	-0.402170	1.392054	1.326028
N	-0.418641	-1.597391	0.105375
N	3.353832	-0.236187	-0.076912
C	1.376787	-0.816733	-1.328138
C	2.581060	0.077785	-1.122943
C	2.839414	1.166945	-1.953619
H	2.155828	1.403388	-2.762680
C	3.955674	1.955251	-1.685958
H	4.184101	2.815250	-2.308073
C	4.760073	1.635928	-0.595893
H	5.632827	2.228240	-0.343801
C	4.413077	0.530968	0.180612
H	5.005523	0.250979	1.048277
C	-0.216070	-2.337660	1.406734
C	-1.553156	-2.727734	2.043361
H	-2.047539	-1.877723	2.525758
H	-1.354302	-3.470882	2.819661
H	-2.239242	-3.175857	1.323763
C	0.567178	-3.607514	1.076884
H	-0.010476	-4.240747	0.395550
H	0.777073	-4.164488	1.995360
H	1.526163	-3.366141	0.619148
C	0.556909	-1.511544	2.465637
H	0.133542	-0.498300	2.496493
H	0.362544	-1.977897	3.438261
C	-1.615211	-0.740883	-0.066796
H	-2.284328	-0.849812	0.794101
C	-2.455142	-1.171981	-1.324782
C	-2.899509	-2.627115	-1.122224
H	-2.038442	-3.280168	-0.946745
H	-3.415950	-2.977996	-2.021894
H	-3.597300	-2.719333	-0.282202
C	-1.658944	-1.098607	-2.632151
H	-1.288780	-0.086941	-2.820873
H	-2.314922	-1.384848	-3.461592
H	-0.820221	-1.800016	-2.618830

C	-3.718529	-0.310007	-1.476203
H	-4.273150	-0.231913	-0.535291
H	-4.371322	-0.771567	-2.224732
H	-3.484330	0.703842	-1.812150
C	-2.796712	3.077581	0.369485
H	-2.400064	3.492968	-0.563290
H	-2.216263	3.476977	1.209811
C	-4.273108	3.373410	0.526501
H	-4.835487	2.947914	-0.308776
H	-4.439957	4.453857	0.546543
H	-4.652870	2.943654	1.456746
C	0.974643	1.818997	1.332923
H	1.324185	1.917200	0.301664
H	1.554491	1.035962	1.830756
C	1.063904	3.139169	2.069747
H	0.504291	3.914717	1.538611
H	2.109667	3.453820	2.138262
H	0.661573	3.045463	3.081891
C	1.786532	-2.211200	-1.773703
H	2.584972	-2.595861	-1.133721
H	0.931787	-2.890907	-1.733978
H	2.155207	-2.165012	-2.803128
H	0.714246	-0.343814	-2.057613

#### RR/SS- 4- Conf A

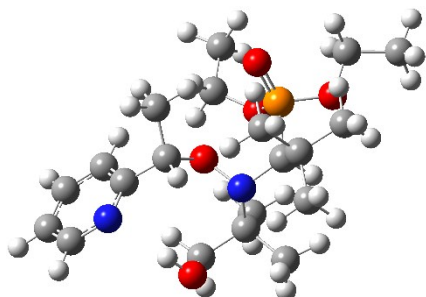


ZPE = 0.550053  
E = -1610.301356  
H = -1610.300412  
G = -1610.396737

P	-1.661199	-0.472248	-0.486096
O	0.942029	-0.167891	0.120365
O	-0.607845	2.127112	-2.206561
H	-0.916775	1.226791	-2.402821
O	-1.066196	-0.515001	-1.853459
O	-1.585347	-1.825094	0.356484
O	-3.263827	-0.260138	-0.577075
N	0.385938	1.062626	0.578734
N	4.364260	-0.651254	0.981168
C	1.943351	-0.742272	0.969142
H	2.061897	-0.120266	1.861381
C	3.268393	-0.800258	0.235196
C	3.307166	-1.057371	-1.139782
H	2.376252	-1.166651	-1.689031

C	4.545460	-1.138430	-1.762865
H	4.614469	-1.327432	-2.829994
C	5.696974	-0.971517	-0.994695
H	6.685514	-1.023853	-1.437859
C	5.549991	-0.736402	0.368925
H	6.423357	-0.605441	1.003751
C	1.524041	-2.168617	1.319018
H	0.589772	-2.179700	1.879456
H	2.312869	-2.649823	1.904105
H	1.379370	-2.736181	0.393514
C	0.915365	2.185249	-0.267774
C	0.261489	3.504717	0.149543
H	-0.810219	3.535512	-0.052955
H	0.715249	4.305228	-0.441986
H	0.441793	3.716933	1.205514
C	2.418591	2.293858	0.013839
H	2.612469	2.226604	1.088784
H	2.792647	3.256119	-0.347139
H	2.985288	1.510084	-0.492338
C	0.732901	1.976760	-1.778255
H	1.344746	2.729925	-2.292529
H	1.111468	0.983227	-2.044920
C	-1.077867	0.870883	0.642597
H	-1.562083	1.742964	0.183604
C	-1.595516	0.819431	2.123936
C	-0.920778	-0.273647	2.955477
H	-1.174840	-1.270541	2.591359
H	-1.259647	-0.191954	3.994154
H	0.165638	-0.149649	2.949714
C	-3.117289	0.624615	2.183670
H	-3.643062	1.348626	1.550545
H	-3.450303	0.773468	3.216223
H	-3.418994	-0.377576	1.869651
C	-1.264580	2.170373	2.774558
H	-0.184378	2.336490	2.794628
H	-1.630678	2.175037	3.806432
H	-1.740024	3.002690	2.243592
C	-2.079172	-3.043140	-0.242899
H	-1.310461	-3.796969	-0.054595
H	-2.167775	-2.908073	-1.326294
C	-3.403734	-3.417990	0.390632
H	-3.288232	-3.531304	1.472045
H	-3.763397	-4.365326	-0.021669
H	-4.147064	-2.640998	0.196328
C	-3.801990	0.642492	-1.562666
H	-3.095198	1.460688	-1.750658
H	-4.698396	1.067479	-1.102576
C	-4.133316	-0.100812	-2.842194
H	-3.222254	-0.512461	-3.282483
H	-4.600405	0.578981	-3.560895
H	-4.829405	-0.917953	-2.632373

**RR/SS- 4- Conf B**



ZPE = 0.550836

E = 1610.301139

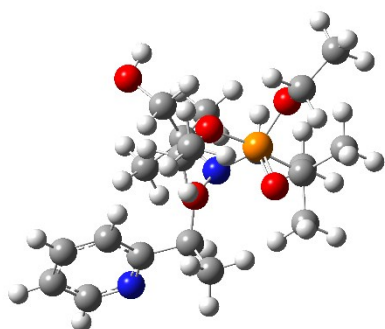
H = -1610.300194

G = -1610.395771

P	-1.981661	0.606631	-0.192932
O	0.719622	0.212821	-0.181041
O	2.729195	-2.360938	0.932794
H	3.123092	-1.997664	0.125311
O	-1.996714	1.163110	-1.570660
O	-3.434102	0.316031	0.444142
O	-1.395616	1.636058	0.896668
N	0.221516	-1.044169	0.287627
N	4.013215	-0.420620	-0.858431
C	1.667788	0.077509	-1.255090
H	1.718157	-0.979357	-1.528063
C	3.046065	0.498632	-0.783101
C	3.271839	1.786135	-0.283365
H	2.450623	2.494219	-0.225476
C	4.545647	2.121615	0.153499
H	4.748890	3.109548	0.555607
C	5.558687	1.166538	0.069479
H	6.569195	1.383026	0.397859
C	5.240803	-0.086108	-0.442132
H	5.995557	-0.864780	-0.515685
C	1.213454	0.934440	-2.431330
H	0.176597	0.715823	-2.687837
H	1.861853	0.747245	-3.292620
H	1.280388	1.999101	-2.186294
C	0.671363	-1.246769	1.700232
C	0.238298	-0.126466	2.650073
H	0.597315	0.842572	2.294215
H	0.652122	-0.311755	3.646684
H	-0.849942	-0.068390	2.742175
C	0.169996	-2.601232	2.211745
H	-0.918581	-2.657824	2.288626
H	0.571157	-2.749274	3.219028
H	0.534088	-3.411781	1.579608
C	2.209573	-1.313702	1.716614
H	2.624195	-0.340540	1.429315
H	2.506878	-1.493092	2.757839
C	-1.237543	-1.067940	0.059074
H	-1.733428	-1.413901	0.973619
C	-1.653954	-2.078502	-1.068224
C	-1.059978	-1.729842	-2.436955
H	-1.413007	-0.760805	-2.796246

H	-1.363546	-2.496577	-3.158501
H	0.032546	-1.731263	-2.402369
C	-3.184322	-2.136798	-1.197691
H	-3.665482	-2.312165	-0.229406
H	-3.451029	-2.960008	-1.868654
H	-3.595363	-1.214148	-1.618664
C	-1.148341	-3.470857	-0.670398
H	-0.060835	-3.470585	-0.558834
H	-1.416803	-4.189674	-1.451745
H	-1.599168	-3.812124	0.268093
C	-4.449677	1.319721	0.278479
H	-4.523774	1.574223	-0.784494
H	-4.149951	2.216343	0.834609
C	-5.749071	0.751364	0.807771
H	-6.023559	-0.148161	0.250825
H	-6.550861	1.487177	0.701048
H	-5.650760	0.490906	1.864530
C	-0.605576	2.760635	0.486057
H	-0.164572	2.559646	-0.493524
H	0.197038	2.847467	1.225776
C	-1.470379	4.005441	0.445864
H	-2.243519	3.895457	-0.320014
H	-0.862819	4.881597	0.199441
H	-1.948025	4.174021	1.414988

#### RR/SS- 4- Conf C

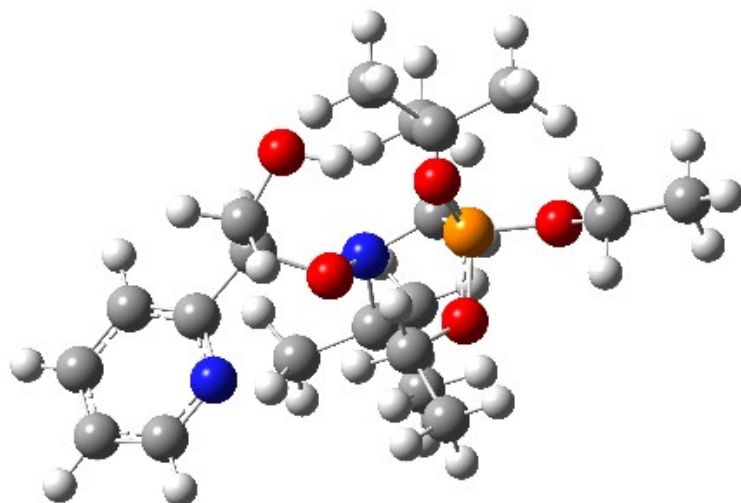


ZPE = 0.549736  
E = -1610.294114  
H = -1610.293170  
G = -1610.390628

P	-1.871954	0.637605	-0.314353
O	0.804547	0.053012	-0.286544
O	0.788345	-0.322123	3.859599
H	0.203996	-0.890775	4.370783
O	-1.854869	1.157532	-1.705260
O	-3.338460	0.455229	0.333066
O	-1.213347	1.647269	0.751561
N	0.216554	-1.147646	0.218980
N	4.166394	-0.578575	-1.230790
C	1.780828	-0.173751	-1.319413
H	1.794514	-1.240596	-1.553861
C	3.166954	0.218323	-0.849168
C	3.367583	1.386761	-0.106892
H	2.512436	1.991368	0.179925
C	4.659679	1.723710	0.271573

H	4.849615	2.617203	0.858697
C	5.709201	0.891126	-0.115062
H	6.735672	1.110777	0.157528
C	5.408188	-0.239641	-0.867700
H	6.198232	-0.912189	-1.193429
C	1.407618	0.667991	-2.536902
H	0.380261	0.476724	-2.847287
H	2.096701	0.444275	-3.356576
H	1.499923	1.733420	-2.301023
C	0.662787	-1.350824	1.633712
C	0.067806	-2.657381	2.170098
H	-1.023246	-2.643102	2.248159
H	0.472064	-2.832925	3.170845
H	0.361358	-3.503261	1.545189
C	2.185875	-1.503655	1.635079
H	2.497802	-2.195844	0.846099
H	2.512503	-1.890222	2.602438
H	2.683570	-0.545583	1.482808
C	0.267253	-0.174114	2.546193
H	0.695094	0.746653	2.143350
H	-0.822789	-0.047309	2.574965
C	-1.240314	-1.077101	-0.019760
H	-1.764259	-1.374604	0.896002
C	-1.714871	-2.077362	-1.133458
C	-1.059597	-1.808484	-2.491357
H	-1.324301	-0.820173	-2.873280
H	-1.407039	-2.560685	-3.208308
H	0.028088	-1.896257	-2.425220
C	-3.241613	-2.012533	-1.299819
H	-3.758303	-2.126495	-0.340769
H	-3.559583	-2.825502	-1.960735
H	-3.563781	-1.069301	-1.750971
C	-1.342894	-3.498960	-0.694176
H	-0.260485	-3.599938	-0.579097
H	-1.673936	-4.211471	-1.456870
H	-1.827341	-3.769961	0.250796
C	-4.287709	1.519510	0.150334
H	-4.304613	1.799673	-0.908642
H	-3.959049	2.384922	0.738374
C	-5.637984	1.015889	0.613887
H	-5.937839	0.144195	0.026499
H	-6.392964	1.797168	0.491115
H	-5.599114	0.729298	1.667793
C	-0.383059	2.731402	0.306010
H	0.118923	2.446377	-0.621889
H	0.366521	2.865240	1.092272
C	-1.217569	3.981832	0.112291
H	-1.943965	3.823213	-0.689945
H	-0.576254	4.824267	-0.163717
H	-1.748448	4.237121	1.033738

**RS/SR-6-conf A**

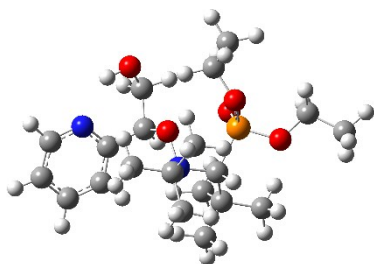


ZPE = 0.551235  
 E = -1610.303261  
 H = -1610.302317  
 G = -1610.396752

C	-1.767948	-0.359412	-1.126104
H	-1.700234	-1.424050	-1.372310
C	-3.148372	-0.013826	-0.607842
C	-4.493829	1.563735	0.363977
H	-4.568595	2.556910	0.801229
C	-5.618639	0.744957	0.281122
H	-6.575416	1.089721	0.657602
C	-5.475027	-0.512061	-0.299347
H	-6.324402	-1.182658	-0.387946
C	-4.218731	-0.897380	-0.754954
H	-4.057540	-1.873928	-1.201985
C	-1.539273	0.500876	-2.380261
H	-2.416251	0.378555	-3.026963
H	-1.518104	1.551509	-2.053574
C	1.294024	-1.042720	0.318464
H	1.794744	-1.141208	1.288505
C	1.863714	-2.197479	-0.581703
C	1.247862	-2.222084	-1.981641
H	1.596255	-3.119164	-2.505798
H	1.533692	-1.350964	-2.570858
H	0.157270	-2.263177	-1.937898
C	1.546672	-3.534925	0.100986
H	0.467322	-3.675311	0.202041
H	2.008484	-3.607837	1.091644
H	1.940722	-4.352034	-0.512064
C	3.390728	-2.085213	-0.714221
H	3.879520	-2.008608	0.263150
H	3.687195	-1.218982	-1.312792
H	3.765177	-2.982631	-1.217746
C	-0.611832	-1.111629	1.958725
C	0.020255	-2.293159	2.706644
H	-0.252771	-3.244654	2.244504
H	-0.365148	-2.288131	3.730016
H	1.109013	-2.236639	2.776071

C	-2.127787	-1.322161	1.998462
H	-2.665490	-0.417046	1.717951
H	-2.428134	-1.581334	3.018212
H	-2.422808	-2.140498	1.333335
C	-0.272408	0.197761	2.677352
H	0.805794	0.369791	2.748076
H	-0.676836	0.158630	3.694245
H	-0.723447	1.045779	2.156639
C	4.234310	1.662841	0.025407
H	4.280158	1.705245	-1.067952
H	3.854358	2.620653	0.399691
C	5.581253	1.328449	0.628876
H	5.509371	1.272709	1.717899
H	6.311886	2.097907	0.364717
H	5.936470	0.365451	0.252945
C	0.178184	2.700997	0.093735
H	-0.810299	2.255817	0.240397
H	0.359127	2.816915	-0.979881
C	0.319697	4.017379	0.828357
H	0.170877	3.872854	1.902056
H	-0.431260	4.724907	0.465560
H	1.311631	4.449137	0.669745
N	-0.168990	-1.148877	0.520150
O	-0.746833	-0.036724	-0.176565
O	-0.416891	0.148090	-3.127038
H	0.388037	0.467268	-2.675346
O	1.825996	0.915921	-1.702985
O	3.316638	0.623783	0.409748
O	1.168028	1.799933	0.632177
P	1.843616	0.637144	-0.236754
N	-3.284900	1.205195	-0.071679

### RS/SR-6-conf B



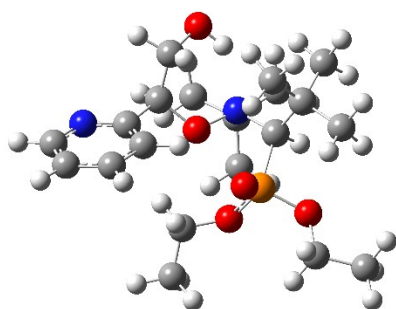
ZPE = 0.551420  
E = -1610.301290  
H = -1610.300346  
G = -1610.394815

C	-1.439206	0.538875	-1.178363
H	-1.002409	-0.201851	-1.854275
C	-2.873355	0.152841	-0.863758
C	-4.961826	0.833880	-0.177997
H	-5.599033	1.667801	0.105615
C	-5.458732	-0.467587	-0.188250
H	-6.487521	-0.662964	0.093758
C	-4.602805	-1.492988	-0.577256
H	-4.948083	-2.521953	-0.608021



C	-3.292341	-1.178177	-0.921047
H	-2.592501	-1.952429	-1.213587
C	-1.307949	1.898796	-1.863565
H	-0.260198	2.022172	-2.151052
H	-1.916951	1.871386	-2.779721
C	0.941990	-1.096031	0.339490
H	1.460930	-1.315848	1.281110
C	0.987937	-2.432068	-0.493022
C	0.401098	-2.312944	-1.905743
H	0.595332	-3.246888	-2.444886
H	0.842732	-1.486871	-2.468888
H	-0.682931	-2.184659	-1.870820
C	0.183842	-3.503195	0.256182
H	-0.849669	-3.180298	0.408675
H	0.626991	-3.738392	1.229681
H	0.174179	-4.423646	-0.337375
C	2.435105	-2.938441	-0.621699
H	2.960859	-2.919159	0.338695
H	3.014742	-2.344250	-1.331934
H	2.413315	-3.972006	-0.982840
C	-0.732687	-0.409225	2.105199
C	-0.598270	-1.731166	2.866359
H	-1.275464	-2.489058	2.465339
H	-0.866740	-1.552125	3.911570
H	0.419665	-2.129993	2.859058
C	-2.186943	0.054441	2.228951
H	-2.334947	1.025382	1.752634
H	-2.438737	0.149259	3.289680
H	-2.869677	-0.671988	1.776350
C	0.174235	0.649327	2.746061
H	1.231471	0.370662	2.719623
H	-0.115676	0.775685	3.794149
H	0.062998	1.609450	2.237375
C	4.572015	0.404149	-0.518159
H	4.476886	0.524656	-1.602842
H	4.588248	1.397279	-0.053392
C	5.804256	-0.396236	-0.152977
H	5.874817	-0.515719	0.931076
H	6.703401	0.114706	-0.508231
H	5.761898	-1.388272	-0.610311
C	1.357382	2.809940	0.140260
H	0.273925	2.748523	0.264635
H	1.573602	2.976127	-0.920012
C	1.966960	3.889064	1.009479
H	1.770889	3.684850	2.065934
H	1.526228	4.856869	0.754916
H	3.049205	3.946550	0.862978
N	-0.440908	-0.643681	0.646784
O	-0.638979	0.619282	0.004544
O	-1.660391	2.990319	-1.043606
H	-2.547564	2.799322	-0.701068
O	1.758693	0.556507	-1.847580
O	3.426600	-0.312351	-0.028725
O	1.949307	1.555751	0.542024
P	1.967447	0.264000	-0.404927
N	-3.706519	1.141123	-0.507332

## RS/SR-6-conf C

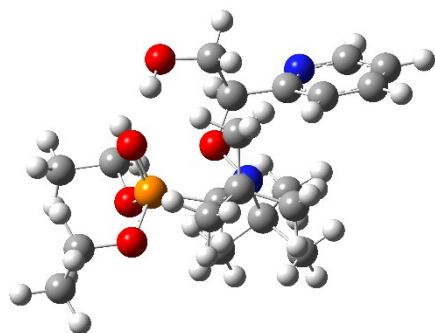


ZPE = 0.551853  
E = -1610.296035  
H = -1610.295091  
G = -1610.389452

C	-2.119373	-1.112694	0.079141
H	-2.557492	-1.561866	0.971778
C	-2.977460	0.075174	-0.297927
C	-2.531655	1.017464	-1.229118
H	-1.521158	0.963910	-1.625200
C	-3.392631	2.049866	-1.585085
H	-3.073399	2.804428	-2.297843
C	-4.660622	2.098360	-1.011060
H	-5.365958	2.884378	-1.259164
C	-5.008921	1.106189	-0.097664
H	-5.988857	1.108210	0.374049
C	-2.170852	-2.130900	-1.058072
H	-3.223673	-2.405814	-1.182102
H	-1.844215	-1.648462	-1.989274
C	1.440551	-0.800235	-0.135585
H	2.301861	-0.943482	0.525530
C	1.878874	-1.370988	-1.530263
C	0.753741	-1.347671	-2.569701
H	1.178506	-1.569145	-3.555004
H	0.270406	-0.368392	-2.622021
H	0.014694	-2.121924	-2.360648
C	2.333450	-2.824989	-1.343653
H	1.539972	-3.450308	-0.925941
H	3.211672	-2.892328	-0.691565
H	2.605651	-3.244835	-2.317614
C	3.078706	-0.582028	-2.084681
H	3.884471	-0.494841	-1.349031
H	2.791843	0.425036	-2.401193
H	3.465536	-1.112035	-2.960962
C	0.500098	-1.932442	1.900138
C	1.543507	-3.055816	1.882945
H	1.205440	-3.895001	1.267877
H	1.681313	-3.418730	2.905310
H	2.520574	-2.728868	1.519135
C	-0.799963	-2.521087	2.457926
H	-1.529821	-1.737303	2.673346
H	-0.574735	-3.025589	3.401962
H	-1.240827	-3.251616	1.773517
C	0.952066	-0.806341	2.835796

H	1.904324	-0.356854	2.539667
H	1.077366	-1.221622	3.840726
H	0.203758	-0.013132	2.879790
C	3.226400	2.780446	-0.179212
H	2.803330	3.142566	-1.122467
H	2.822224	3.382590	0.643279
C	4.739629	2.814931	-0.199683
H	5.144482	2.433504	0.740989
H	5.090030	3.840991	-0.341057
H	5.120952	2.199695	-1.018858
C	-0.618898	2.202817	1.332067
H	-1.295407	1.417123	1.684050
H	-0.960834	2.538950	0.349300
C	-0.527650	3.348327	2.318499
H	-0.152505	2.995685	3.283110
H	-1.517802	3.787656	2.469112
H	0.146033	4.124876	1.946394
N	0.280655	-1.507290	0.465361
O	-0.815464	-0.576382	0.388006
O	-1.455347	-3.316448	-0.796806
H	-0.583835	-3.029030	-0.473996
O	0.627574	1.643000	-1.384496
O	2.824558	1.413578	0.014793
O	0.694398	1.632674	1.203312
P	1.265348	1.052176	-0.178691
N	-4.191209	0.112614	0.260073

### RR/SS-6- Conf A



ZPE = 0.550960

E = -1610.294571

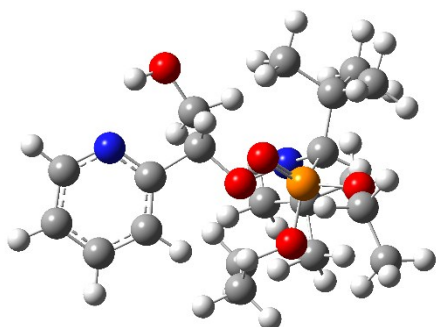
H = -1610.293627

G = -1610.387831

C	1.610639	-1.314147	-0.718962
H	1.618250	-2.368235	-0.421676
C	2.991201	-0.775539	-0.411729
C	5.125585	-1.312979	0.240120
H	5.807485	-2.094596	0.566807
C	5.567569	0.001108	0.106368
H	6.595854	0.260263	0.334329
C	4.654659	0.955748	-0.331323
H	4.952728	1.992159	-0.458810
C	3.349240	0.562679	-0.603121
H	2.606455	1.282665	-0.918514

C	1.352934	-1.272678	-2.229516
H	1.401235	-0.242341	-2.598949
H	2.173054	-1.826634	-2.701432
C	-0.709225	1.199764	0.197619
H	-1.146637	1.655639	1.092606
C	-1.697182	-2.581274	0.215201
H	-1.238052	-2.544936	-0.774656
H	-0.927492	-2.867902	0.939111
C	-2.882841	-3.523300	0.245763
H	-3.342691	-3.540210	1.237939
H	-2.560209	-4.537468	-0.006276
H	-3.633858	-3.209025	-0.485126
C	-4.621634	0.288000	-0.156725
H	-5.205990	1.110304	-0.578043
H	-4.532083	-0.490251	-0.922774
C	-5.244572	-0.245880	1.117768
H	-4.629570	-1.049621	1.529026
H	-6.246388	-0.634482	0.911709
H	-5.326903	0.549194	1.863325
C	0.723784	0.395694	2.085338
C	-0.460746	-0.273564	2.796229
H	-1.410739	0.246509	2.643108
H	-0.260600	-0.284294	3.872103
H	-0.582410	-1.303889	2.458714
C	0.948250	1.799821	2.656071
H	1.798072	2.285310	2.168866
H	1.171379	1.709266	3.723189
H	0.072681	2.447453	2.561295
C	1.976616	-0.428659	2.392510
H	1.916075	-1.433873	1.968517
H	2.064900	-0.527602	3.478660
H	2.881763	0.060528	2.024437
C	-0.522059	2.388320	-0.812054
C	0.068785	1.973094	-2.161341
H	0.079643	2.844481	-2.825390
H	-0.515528	1.183250	-2.638496
H	1.101227	1.640456	-2.051319
C	0.421530	3.415686	-0.172401
H	1.384550	2.963830	0.080203
H	-0.007997	3.848913	0.737355
H	0.599071	4.231986	-0.880428
C	-1.869632	3.083397	-1.069989
H	-2.390441	3.321045	-0.136679
H	-2.534628	2.470847	-1.684877
H	-1.683182	4.018737	-1.607853
N	0.555677	0.525230	0.586159
O	0.489017	-0.793019	0.033908
O	0.156058	-1.903589	-2.594640
H	-0.598426	-1.309766	-2.418979
O	-2.016389	-0.345475	-1.804917
O	-2.155129	-1.269027	0.599123
O	-3.318012	0.835442	0.128572
P	-2.026221	0.010277	-0.355141
N	3.873027	-1.699268	-0.009762

**RR/SS-6- Conf B**

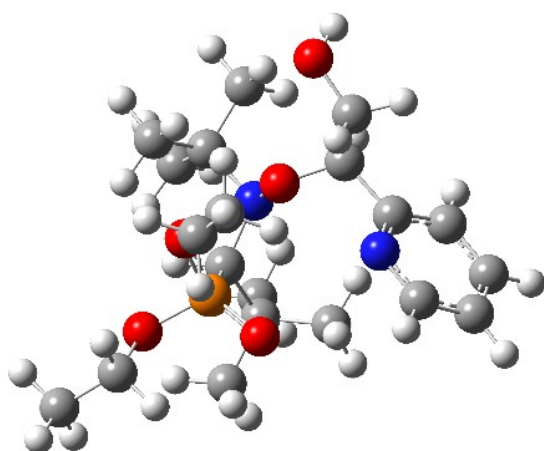


ZPE = 0.551427  
 E = -1610.296452  
 H = -1610.295508  
 G = -1610.391491

C	-1.700444	-0.657157	-0.508405
H	-1.254606	-0.508030	-1.499527
C	-2.846661	0.319943	-0.356361
C	-4.799229	1.081585	-1.298417
H	-5.484482	1.027983	-2.140642
C	-5.055914	1.931396	-0.225952
H	-5.940745	2.557975	-0.222535
C	-4.153409	1.938908	0.833376
H	-4.322451	2.574695	1.697572
C	-3.032285	1.116637	0.775420
H	-2.306931	1.081452	1.580022
C	-2.267037	-2.089922	-0.437515
H	-1.452455	-2.790597	-0.245674
H	-2.989595	-2.163447	0.389803
C	1.491413	-1.004529	0.035857
H	2.320369	-1.095755	0.748929
C	0.054998	2.607618	0.656586
H	-0.654495	2.214339	-0.074396
H	-0.413524	2.602262	1.646204
C	0.513168	3.999907	0.269880
H	1.251046	4.379919	0.981806
H	-0.340591	4.684178	0.255808
H	0.954319	3.984359	-0.731003
C	3.734756	2.193044	-0.912641
H	4.526778	1.940461	-1.623141
H	2.972195	2.766976	-1.451210
C	4.277612	2.956428	0.279294
H	3.474922	3.162173	0.991523
H	4.715537	3.904374	-0.047702
H	5.050149	2.371878	0.785472
C	0.292594	-1.531110	2.213246
C	0.678687	-0.246046	2.955242
H	1.678872	0.101484	2.681382
H	0.664934	-0.433197	4.033675
H	-0.028261	0.556203	2.730409
C	1.286039	-2.643040	2.563759
H	1.021377	-3.582120	2.073038
H	1.251372	-2.802065	3.645524
H	2.319117	-2.392894	2.308312
C	-1.095288	-1.991177	2.672821

H	-1.856526	-1.234747	2.467512
H	-1.078272	-2.175640	3.751016
H	-1.377498	-2.920610	2.169145
C	1.823091	-1.989729	-1.146205
C	0.769333	-1.991628	-2.261096
H	1.115434	-2.652716	-3.063336
H	0.622260	-0.993554	-2.681202
H	-0.190391	-2.384785	-1.918117
C	1.908595	-3.410128	-0.572998
H	0.957647	-3.706483	-0.122244
H	2.700916	-3.499534	0.178907
H	2.132579	-4.112080	-1.382834
C	3.185974	-1.648867	-1.770561
H	3.967284	-1.535476	-1.011846
H	3.147617	-0.727650	-2.358250
H	3.474543	-2.462757	-2.443585
N	0.230631	-1.358505	0.725476
O	-0.741180	-0.338096	0.498445
O	-2.853207	-2.446331	-1.667393
H	-3.412523	-1.707692	-1.955758
O	0.884435	1.145890	-1.739608
O	1.184234	1.725491	0.755879
O	3.177142	0.940546	-0.475344
P	1.575303	0.769547	-0.480529
N	-3.723889	0.294951	-1.368751

### RR/SS-6- Conf C

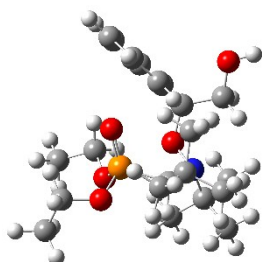


ZPE = 0.549839  
E = -1610.289962  
H = -1610.289017  
G = -1610.384957

C	-2.284207	0.753762	-0.324825
H	-2.689714	1.425071	0.441295
C	-2.667245	-0.681917	-0.021783
C	-2.369856	-2.878154	-0.590050
H	-1.851455	-3.590750	-1.226797
C	-3.255913	-3.310913	0.395755
H	-3.440572	-4.370051	0.538661
C	-3.893088	-2.352439	1.178935

H	-4.596576	-2.646858	1.951972
C	-3.593529	-1.010519	0.968434
H	-4.038314	-0.231273	1.580991
C	-2.864589	1.063794	-1.712698
H	-2.362868	0.407651	-2.428072
H	-3.929214	0.793793	-1.705884
C	0.914182	0.428614	1.043753
H	1.803094	1.044059	1.219825
C	0.430943	-0.063812	-2.775254
H	-0.323654	-0.734588	-2.354654
H	-0.042288	0.887677	-3.039301
C	1.135100	-0.694374	-3.959760
H	1.926068	-0.038980	-4.335256
H	0.420290	-0.876021	-4.768266
H	1.576813	-1.651529	-3.666826
C	3.911904	-1.390773	-0.858083
H	3.531195	-2.414669	-0.775509
H	3.881131	-1.089722	-1.912447
C	5.310071	-1.269137	-0.290116
H	5.666201	-0.238732	-0.366649
H	5.996873	-1.918745	-0.839939
H	5.317774	-1.563479	0.762701
C	0.157396	2.785163	0.629819
C	1.047374	3.022173	-0.594545
H	2.000011	2.488193	-0.520345
H	1.264943	4.091923	-0.679226
H	0.540416	2.694089	-1.504466
C	0.863524	3.288728	1.893943
H	0.238150	3.154629	2.779717
H	1.048664	4.359550	1.768435
H	1.832590	2.817226	2.073796
C	-1.129676	3.600198	0.484046
H	-1.628583	3.363325	-0.454968
H	-0.882128	4.666038	0.476993
H	-1.802500	3.410000	1.327621
C	0.743721	-0.446212	2.334331
C	-0.505576	-1.324798	2.274206
H	-0.539427	-1.966224	3.162519
H	-0.510737	-1.960022	1.384097
H	-1.399633	-0.698697	2.281857
C	0.608328	0.481914	3.548105
H	-0.259519	1.138331	3.442002
H	1.503653	1.096684	3.693598
H	0.468008	-0.123769	4.450124
C	1.982530	-1.329796	2.555962
H	2.905019	-0.739490	2.544943
H	2.065604	-2.113931	1.797987
H	1.896011	-1.814248	3.534290
N	-0.233106	1.338451	0.800061
O	-0.874068	0.936499	-0.419645
O	-2.673683	2.387966	-2.163639
H	-3.347442	2.958741	-1.779227
O	0.930121	-1.973113	-0.522434
O	1.409611	0.248435	-1.764617
O	3.057005	-0.516629	-0.104969
P	1.468751	-0.595113	-0.403431
N	-2.096807	-1.593135	-0.811882

## RR/SS-9-conf C



ZPE = 0.562123

E = -1594.246515

H = -1594.245571

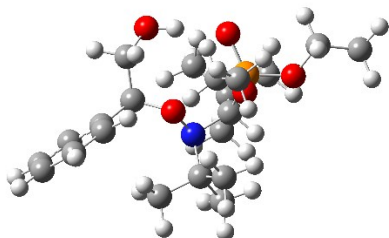
G = -1594.341076

C	-1.497487	-1.114304	-0.541991
H	-1.005239	-0.967506	-1.506521
C	-2.686949	-0.186450	-0.477060
C	-2.982853	0.644786	-1.556639
H	-2.348522	0.612961	-2.437963
C	-4.056468	1.532243	-1.488701
H	-4.278445	2.176816	-2.333658
C	-4.835233	1.600085	-0.335080
H	-5.668380	2.294209	-0.279638
C	-4.542161	0.772193	0.749635
H	-5.145251	0.821388	1.651304
C	-3.474564	-0.118355	0.675221
H	-3.239427	-0.752146	1.527149
C	-1.879666	-2.584711	-0.413438
H	-0.967225	-3.182551	-0.296687
H	-2.518847	-2.736309	0.468018
C	1.670964	-0.726145	-0.054253
H	2.512036	-0.603802	0.640845
C	-0.736931	2.232645	0.881363
H	-1.196647	2.149749	-0.107021
H	-1.266779	1.558682	1.560795
C	-0.745061	3.661542	1.383099
H	-0.254651	3.734608	2.358123
H	-1.776680	4.011177	1.484318
H	-0.224254	4.319330	0.680625
C	2.822548	3.058843	-0.783985
H	3.587399	3.147352	-1.560397
H	1.881037	3.441525	-1.194570
C	3.222476	3.797400	0.478341
H	2.449052	3.684426	1.241759
H	3.359877	4.861843	0.264850
H	4.161759	3.397756	0.869521
C	0.754034	-1.667419	2.108027
C	0.880235	-0.359858	2.899547
H	1.756304	0.221131	2.596100
H	0.980090	-0.592016	3.964637
H	-0.003969	0.265241	2.759720
C	1.992143	-2.533551	2.355940
H	1.913172	-3.496687	1.846744
H	2.067187	-2.721587	3.430996
H	2.921667	-2.048496	2.047432



C	-0.464944	-2.448493	2.608036
H	-1.379397	-1.860160	2.508633
H	-0.329387	-2.694488	3.665473
H	-0.578422	-3.382973	2.049887
C	2.238637	-1.523269	-1.287214
C	1.186461	-1.825431	-2.360629
H	1.674327	-2.352124	-3.188335
H	0.735284	-0.911784	-2.755882
H	0.402030	-2.482763	-1.974840
C	2.783907	-2.866098	-0.783206
H	1.989448	-3.459444	-0.322771
H	3.594069	-2.733151	-0.057918
H	3.182867	-3.433110	-1.630789
C	3.398353	-0.756940	-1.943418
H	4.138692	-0.430482	-1.205853
H	3.049973	0.126703	-2.484947
H	3.893732	-1.418276	-2.661874
N	0.574897	-1.451558	0.633222
O	-0.627061	-0.681507	0.513140
O	-2.563197	-2.907575	-1.611835
H	-2.869316	-3.818653	-1.570682
O	0.401110	1.215010	-1.705692
O	0.632661	1.794085	0.808114
O	2.694971	1.652195	-0.505697
P	1.212269	1.020304	-0.476330

### RS/SR-9-Conf A



ZPE = 0.562256

E = -1594.253395

H = -1594.252451

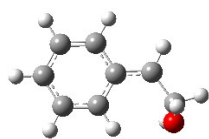
G = -1594.347854

C	-1.783035	-0.217483	-1.112295
H	-1.686456	-1.268158	-1.400147
C	-3.183424	0.057436	-0.610852
C	-3.510156	1.295198	-0.048498
H	-2.733898	2.043789	0.087388
C	-4.810753	1.562909	0.369735
H	-5.048114	2.524342	0.815079
C	-5.806859	0.597431	0.218577
H	-6.820742	0.804158	0.546695
C	-5.493514	-0.631912	-0.357006
H	-6.263095	-1.387818	-0.479585

C	-4.188759	-0.896258	-0.771456
H	-3.944123	-1.860298	-1.211604
C	-1.532378	0.685510	-2.330153
H	-2.413146	0.612958	-2.976875
H	-1.480910	1.727443	-1.971434
C	1.237782	-1.057439	0.305837
H	1.748194	-1.204576	1.264284
C	1.712306	-2.238952	-0.616965
C	1.081313	-2.206270	-2.009873
H	1.399015	-3.098377	-2.561293
H	1.384385	-1.328177	-2.580004
H	-0.008954	-2.222281	-1.956047
C	1.313749	-3.558893	0.056389
H	0.229380	-3.621704	0.179723
H	1.789970	-3.677712	1.035848
H	1.634135	-4.394021	-0.574801
C	3.241761	-2.230627	-0.772211
H	3.750678	-2.188947	0.196747
H	3.587159	-1.386220	-1.376233
H	3.545987	-3.150654	-1.281958
C	-0.631727	-1.021375	1.991007
C	-0.034622	-2.233710	2.719241
H	-0.360422	-3.169487	2.259853
H	-0.398739	-2.216594	3.750204
H	1.056699	-2.227502	2.767913
C	-2.152704	-1.172666	2.066789
H	-2.668968	-0.258966	1.775821
H	-2.438479	-1.403374	3.097524
H	-2.491771	-1.989068	1.421221
C	-0.216494	0.265579	2.710473
H	0.869877	0.383503	2.764688
H	-0.607890	0.243837	3.732745
H	-0.631068	1.138727	2.200426
C	4.369903	1.426342	0.005059
H	4.380697	1.508300	-1.086849
H	4.079600	2.394874	0.429314
C	5.706545	0.963621	0.543576
H	5.669693	0.870072	1.631713
H	6.486021	1.683635	0.279876
H	5.970087	-0.008244	0.118291
C	0.441343	2.771237	0.145990
H	-0.581239	2.445263	0.358244
H	0.573375	2.834464	-0.938915
C	0.762637	4.084450	0.828101
H	0.661146	3.986350	1.912272
H	0.075814	4.861782	0.481315
H	1.785066	4.397483	0.600654
N	-0.223256	-1.063645	0.542589
O	-0.764798	0.078965	-0.135757
O	-0.422582	0.338252	-3.098918
H	0.398477	0.590569	-2.635345
O	1.882621	0.898533	-1.690933
O	3.385666	0.447716	0.385589
O	1.332363	1.773983	0.669824
P	1.908113	0.579452	-0.233473

## Ethyl radicals

### 2-hydroxy-1-phenyl-ethyl radical



$$\langle S^2 \rangle = 0.773086$$

$$\text{ZPE} = 0.144618$$

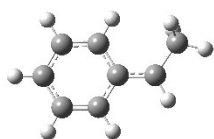
$$E = -385.135267$$

$$H = -385.134323$$

$$G = -385.177622$$

C	0.008128	0.085885	-0.067950
H	-0.031318	0.334986	0.988927
C	1.284538	0.008373	-0.690128
C	1.434240	-0.330027	-2.059790
H	0.547916	-0.489495	-2.665491
C	2.695269	-0.429400	-2.628630
H	2.789529	-0.690190	-3.678435
C	3.842148	-0.190977	-1.865984
H	4.825235	-0.267874	-2.319104
C	3.715356	0.152216	-0.515945
H	4.601740	0.339940	0.082336
C	2.460939	0.251117	0.063503
H	2.365486	0.513075	1.114305
C	-1.275415	-0.203113	-0.779988
H	-1.266394	-1.217414	-1.199135
H	-2.113380	-0.146983	-0.074587
O	-1.510768	0.647498	-1.901134
H	-1.380864	1.561754	-1.622784

### 1-phenyl-ethyl radical



$$\langle S^2 \rangle = 0.774144$$

$$\text{ZPE} = 0.139099$$

$$E = -309.951313$$

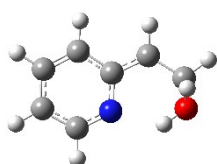
$$H = -309.950369$$

$$G = -309.991108$$

C	0.008794	-0.060898	0.048592
H	0.013298	-0.146456	1.130999
C	1.263470	-0.017572	-0.614650
C	1.365856	0.094758	-2.024768

H	0.462397	0.150466	-2.624520
C	2.604788	0.134642	-2.648394
H	2.657918	0.221021	-3.729657
C	3.781616	0.064844	-1.898607
H	4.747628	0.096479	-2.391830
C	3.704156	-0.046179	-0.505697
H	4.613691	-0.100974	0.085129
C	2.472296	-0.086749	0.125517
H	2.417798	-0.173082	1.207846
C	-1.303691	0.006210	-0.661007
H	-1.405599	0.936920	-1.235783
H	-1.419981	-0.819687	-1.376168
H	-2.135834	-0.043431	0.043318

### 2-hydroxy-1-pyridyl-ethyl radical



$\langle S^2 \rangle = 0.773281$

ZPE = 0.133853

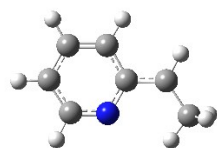
E = -401.187800

H = -401.186856

G = -401.229270

C	0.011685	-0.029885	0.042396
H	-0.022935	-0.069537	1.126627
C	1.284711	-0.019744	-0.589858
C	2.488349	0.089976	-2.558009
H	2.461529	0.152469	-3.643701
C	3.714040	0.045257	-1.888638
H	4.642876	0.073676	-2.446685
C	3.699852	-0.042348	-0.495030
H	4.628839	-0.081956	0.065599
C	2.483203	-0.076544	0.162100
H	2.430194	-0.141908	1.244363
C	-1.266008	0.072157	-0.736324
H	-2.118032	-0.105683	-0.075971
H	-1.362403	1.099847	-1.127061
O	-1.366010	-0.865299	-1.788763
H	-0.596126	-0.711441	-2.357237
N	1.308963	0.058161	-1.949851

### 1-pyridyl-ethyl radical

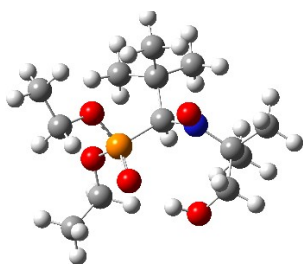


$\langle S^2 \rangle = 0.77419$

ZPE = 0.127709  
 E = -326.000563  
 H = -325.999619  
 G = -326.040809

C	0.030176	0.024197	0.021162
H	0.020040	0.024441	1.107801
C	1.299774	0.006314	-0.616848
C	2.528630	-0.003120	-2.565626
H	2.516938	0.002842	-3.653998
C	3.748513	-0.026089	-1.882422
H	4.683917	-0.038022	-2.430293
C	3.716531	-0.033220	-0.485694
H	4.637529	-0.051031	0.089497
C	2.491402	-0.017024	0.154053
H	2.424915	-0.021571	1.237868
C	-1.267100	0.056588	-0.704652
H	-1.802198	0.994672	-0.506871
H	-1.107380	-0.032098	-1.779602
H	-1.924387	-0.754102	-0.368613
N	1.340515	0.012629	-1.976345

### Nitroxide 3°

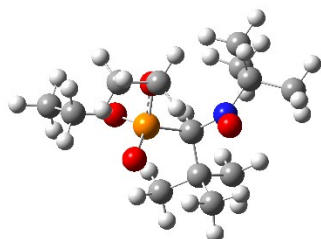


$\langle S^2 \rangle = 0.754795$   
 ZPE = 0.415912  
 E = -1284.240473  
 H = -1284.239529  
 G = -1284.323298

P	-0.355547	-0.132260	0.136927
O	0.146810	0.352274	2.995160
O	3.099034	-0.104660	0.978078
H	2.324106	-0.650544	0.747420
O	0.667470	-1.184436	0.388891
O	-1.854657	-0.538264	0.481146
O	-0.460960	0.248630	-1.427004
N	0.699047	1.200306	2.215483
C	2.124158	1.550291	2.508375
C	2.646235	2.648748	1.587947
H	2.733121	2.302097	0.556185
H	3.653795	2.915392	1.920445
H	2.029009	3.549136	1.632812
C	2.178868	1.995861	3.970832
H	1.569441	2.892219	4.122548

H	3.211009	2.229309	4.246306
H	1.802930	1.207178	4.625374
C	2.976468	0.278044	2.324783
H	3.983745	0.491821	2.701698
H	2.536042	-0.520443	2.935605
C	-0.023974	1.481991	0.976886
H	0.665002	1.977716	0.282677
C	-1.233406	2.452012	1.183130
C	-2.186838	1.986695	2.291056
H	-2.590146	0.993725	2.088371
H	-3.017347	2.698462	2.354654
H	-1.680617	1.955963	3.258438
C	-1.997711	2.606956	-0.139703
H	-1.326470	2.884178	-0.960050
H	-2.744537	3.399659	-0.029355
H	-2.518085	1.688226	-0.420966
C	-0.668881	3.823930	1.578347
H	-0.088646	3.762774	2.504993
H	-1.493047	4.524283	1.746359
H	-0.030580	4.238421	0.789518
C	-2.305131	-1.860710	0.104065
H	-1.599577	-2.592473	0.507059
H	-2.303628	-1.925784	-0.989693
C	-3.694098	-2.041434	0.673648
H	-3.670060	-1.955730	1.762431
H	-4.078820	-3.029593	0.408307
H	-4.373319	-1.283263	0.276369
C	0.741427	0.202935	-2.226730
H	1.615289	0.427490	-1.602840
H	0.624699	0.999472	-2.965210
C	0.886054	-1.156454	-2.881120
H	1.008224	-1.924224	-2.113142
H	1.763439	-1.169043	-3.533834
H	0.000900	-1.382626	-3.481182

### Nitroxide 6°



$\langle S^2 \rangle = 0.754656$   
 ZPE = 0.409605  
 E = -1209.048767  
 H = -1209.047822  
 G = -1209.129238

P	1.599059	0.345928	-0.208899
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O	-1.244973	0.380649	0.452515
N	-0.612175	-0.567865	1.026659
O	3.049270	-0.294727	0.073387
O	1.475722	1.418861	0.981452
O	1.416598	0.916311	-1.564418
H	1.178823	-1.644833	1.013107
C	0.553046	-1.087352	0.310893
C	-0.935767	-0.796660	2.469462
H	-0.431503	-0.488035	-2.248063
H	-1.776837	-1.214472	-1.353047
H	-0.991758	-2.127022	-2.657953
C	0.175741	-2.053524	-0.854450
C	-0.818991	-1.422827	-1.836232
H	1.876896	-1.608045	-2.156592
H	1.219252	-3.241920	-2.323276
H	2.221646	-2.833929	-0.916320
H	-1.285273	1.312867	2.800075
H	0.378971	0.793647	3.150764
H	-0.938884	0.385273	4.279176
C	1.456802	-2.452810	-1.602457
H	-0.063650	2.493933	0.087476
H	0.405849	2.960674	1.736548
C	-0.675215	0.511732	3.224675
H	-1.340023	-3.068444	0.345279
H	0.264038	-3.842354	0.401550
H	-0.753719	-3.998788	-1.039977
C	0.784871	2.668991	0.753577
H	-3.018070	-0.389004	2.046261
H	-2.733979	-1.241299	3.582437
H	-2.612239	-2.119650	2.044035
C	-0.448876	-3.313539	-0.242425
H	4.075140	0.660578	-1.448332
H	4.245932	1.390699	0.166808
C	-2.421812	-1.161072	2.536941
H	6.321982	0.121251	-0.457235
H	5.353024	-1.352012	-0.665847
H	5.522892	-0.621950	0.943912
C	4.199339	0.442688	-0.382739
H	1.234096	4.663736	0.087151
H	2.093094	3.383378	-0.794070
H	2.599952	3.831756	0.857829
C	5.424509	-0.406206	-0.122789
H	0.969666	-1.648186	3.120122
H	-0.193311	-2.851578	2.500116
H	-0.435399	-2.105171	4.083688
C	1.742227	3.700363	0.191612
C	-0.088899	-1.919752	3.063165

## References

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<sup>1</sup> **2**, **2'**, and **2''** differ only by the pathway of preparation as well as **3** and **3'**.

<sup>2</sup> *RS/SR-5* exhibits 3.2 kJ/mol lower  $E_a$  than expected. A tentative rationale is a different conformation in *RS/SR-5* than in *RS/SR-2*

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