

## Microwave-assisted nucleophilic degradation of organophosphate pesticides in Propylene Carbonate

Daniela Millán<sup>1,2\*</sup>, Mabel Rojas<sup>1</sup>, Paulina Pavez<sup>1</sup> and Ricardo A. Tapia<sup>1</sup>

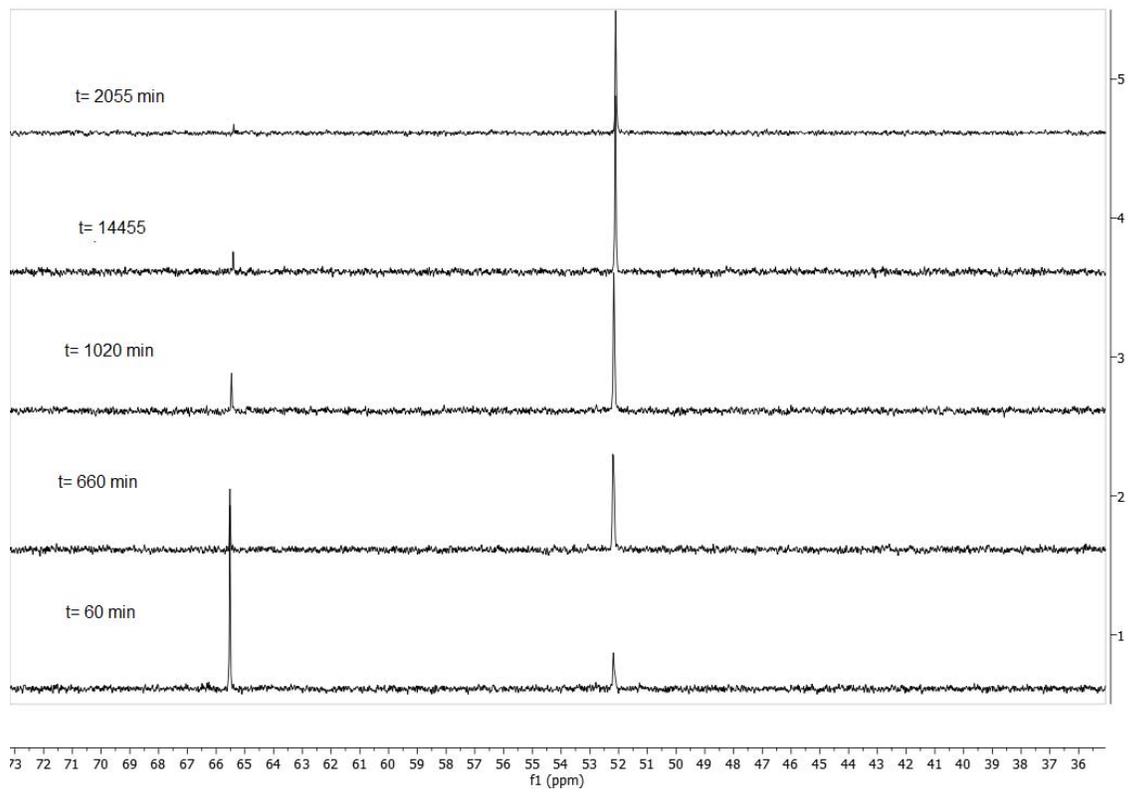
<sup>1</sup>Facultad de Química. Pontificia Universidad Católica de Chile. Casilla 306, Santiago 6094411, Chile.

<sup>2</sup>Universidad Bernardo O'Higgins, Laboratorio de Bionanotecnología, General Gana 1702, Santiago, Chile

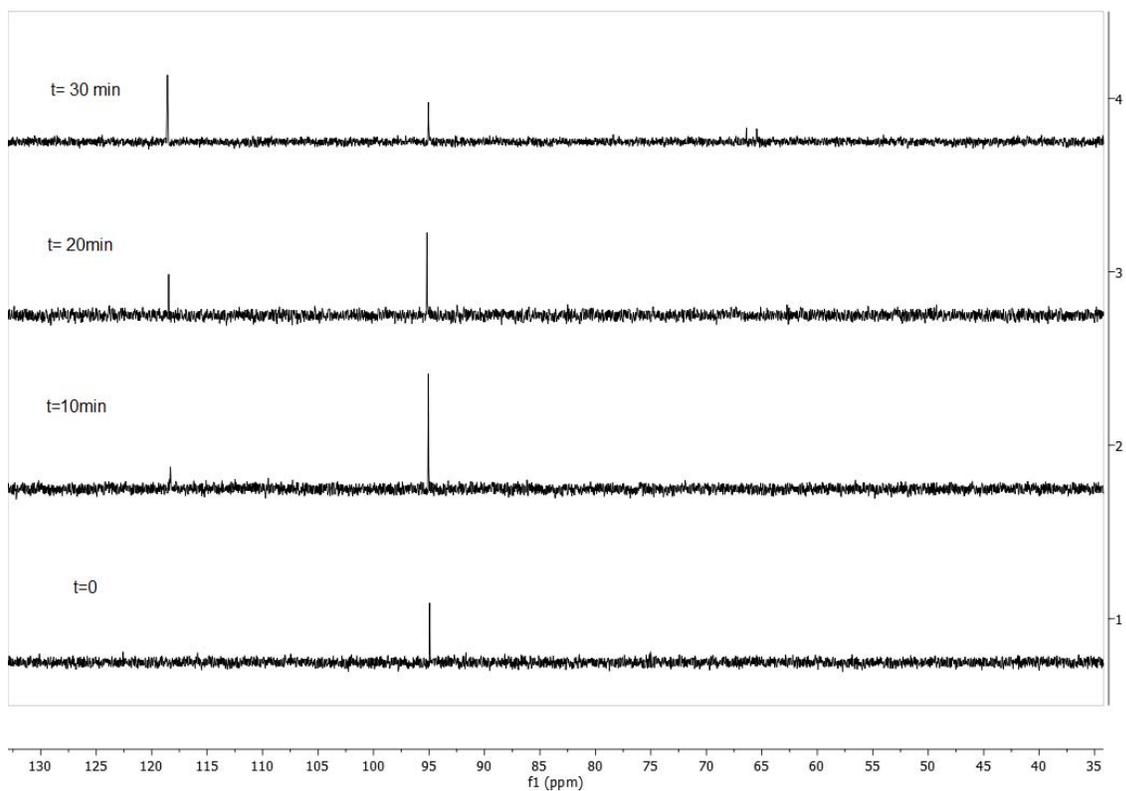
**Table S1:** Pseudo-first-order rate constants ( $k_{\text{obsd}}$ ) and second-order rate constant ( $K_2$ ) for the degradation of pesticides **1-5** in PC at room temperature.

	$10^3 K_{\text{OBS}}/\text{min}^{-1}$		$10^3 K_2/\text{M}^{-1}\text{min}^{-1}$	
	Bmim[Ala]	Piperidine	Bmim[Ala]	Piperidine
Malathion (1)	65.1±4.00	70±4	162.7±10	175±10
Fenitrothion (2)	1.60±0.04	30±1	4.0±0.20	75±2.5
Paraoxon (3)	0.58±0.05	--	1.5±0.08	
Diazinon (4)	--	--		
Parathion (5)	--	--		

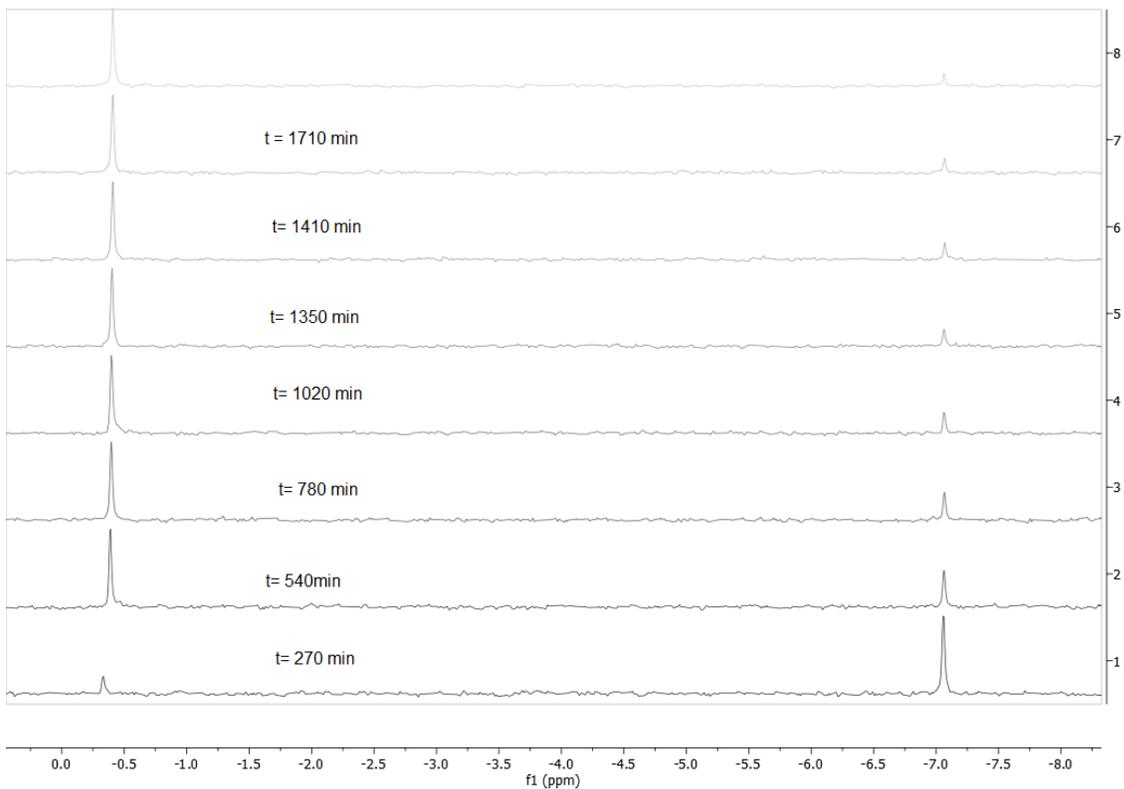
--- not reaction observed. Values are mean and standard deviation (±S.D.) of three independent experiments



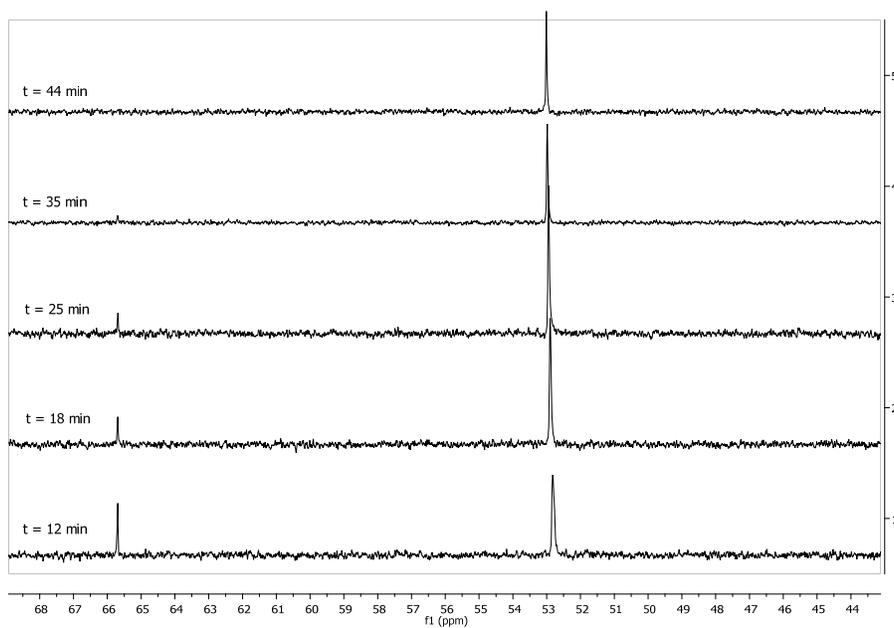
**Figure S1:** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of fenitroion with Bmim[Ala] in propylene carbonate at 25°C.



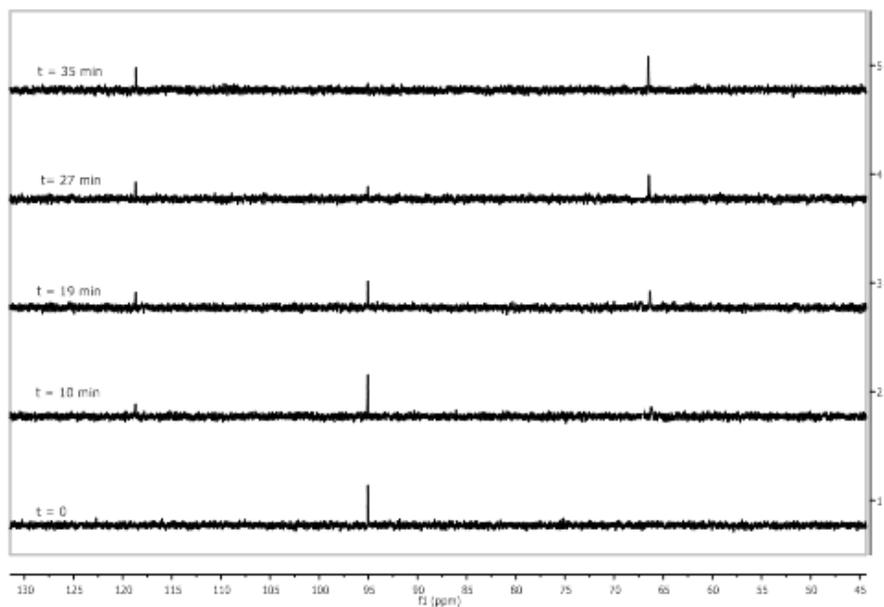
**Figure S2:** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of malathion with Bmim[Ala] in propylene carbonate at  $25^\circ\text{C}$ .



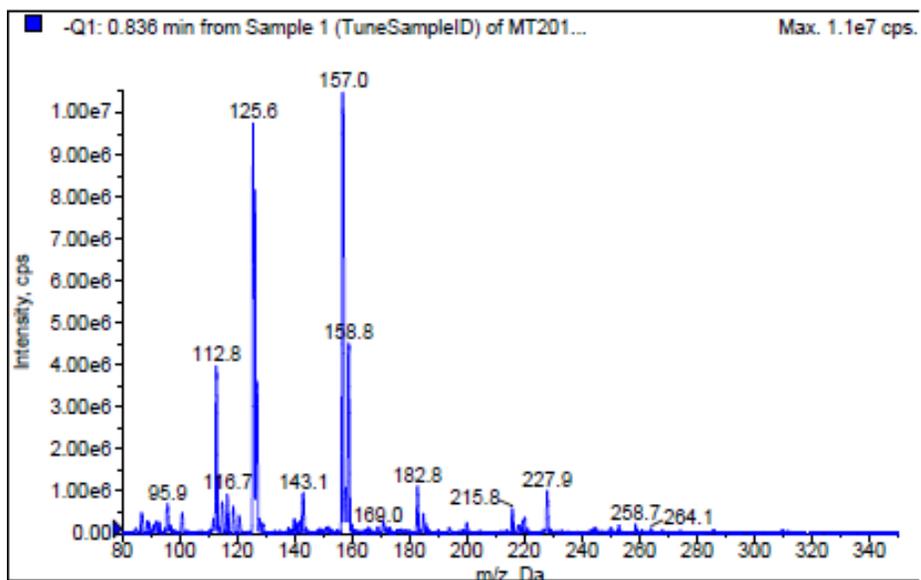
**Figure S3:** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of paraoxon with Bmim[Ala] in propylene carbonate at  $25^\circ\text{C}$ .



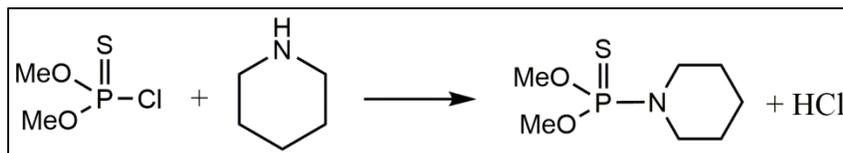
**Figure S4:** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of fenitroton with piperidine in propylene carbonate at  $25^\circ\text{C}$ .



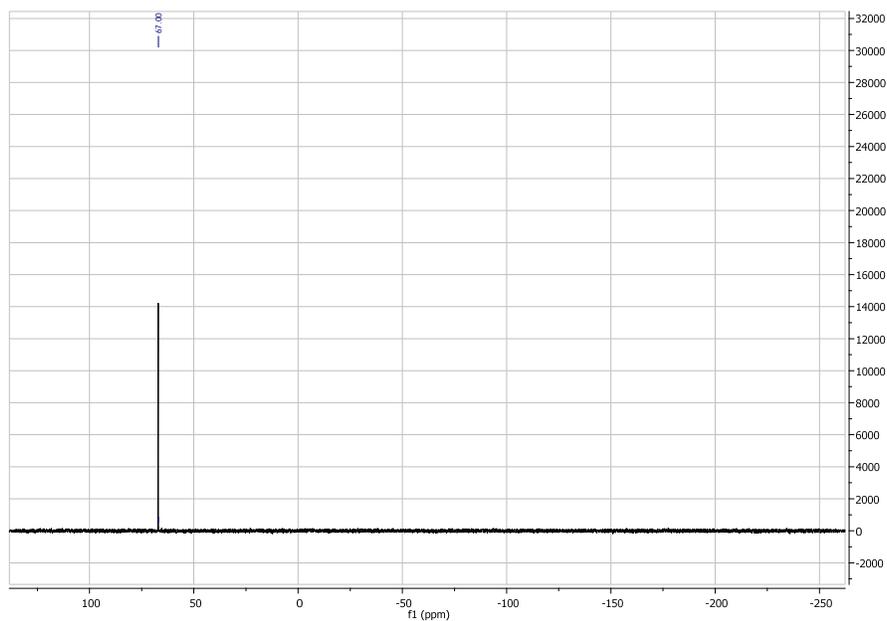
**Figure S5:** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of malathion with piperidine in propylene carbonate at  $25^\circ\text{C}$ .



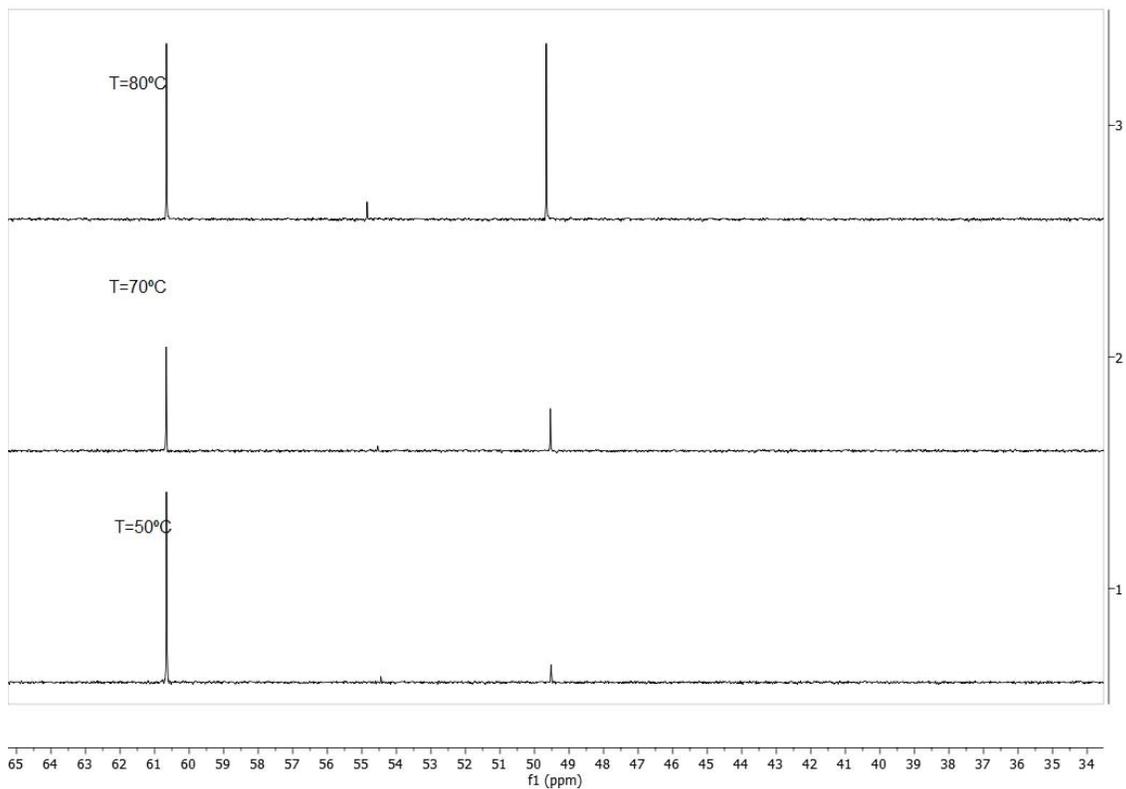
**Figure S6:** ESI-MS/MS(-) of the compound **6** of  $m/z$  157, from a reaction of malathion with piperidine in PC.



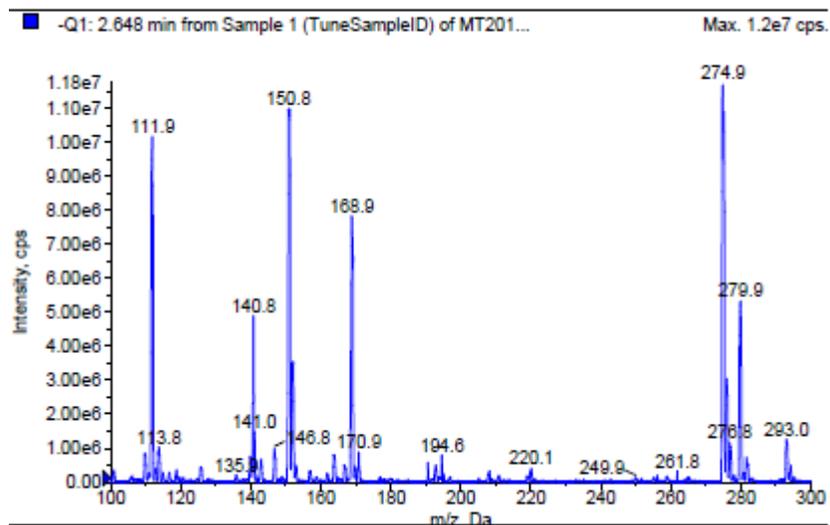
**Scheme S1:** Reaction route to identify product **8**



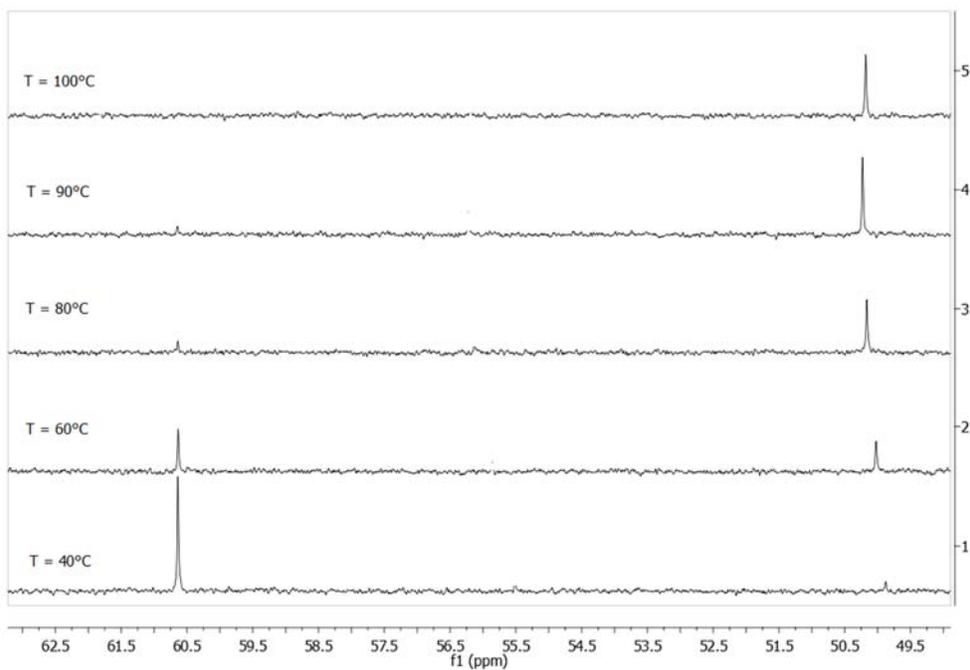
**Figure S7:** <sup>31</sup>P-NMR plot for product **8** obtained from the reaction of *O,O*-dimethyl chlorothiophosphate with piperidine in PC at 25°C.



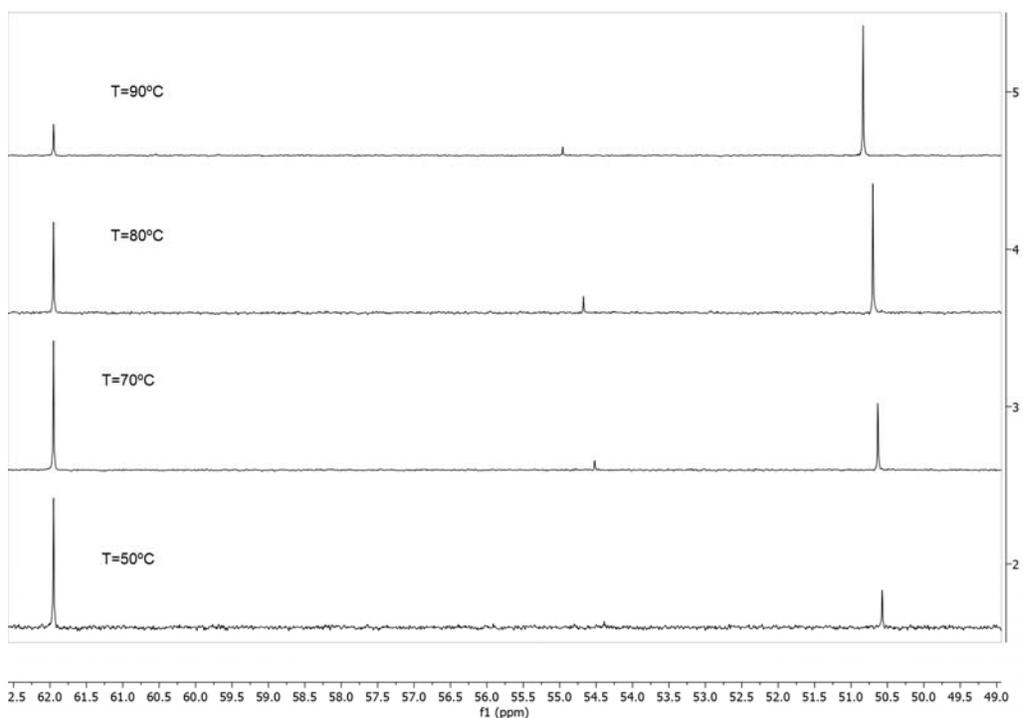
**Figure S8:** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of diazinon with Bmim[Ala] in propylene carbonate at different temperatures under MW heating



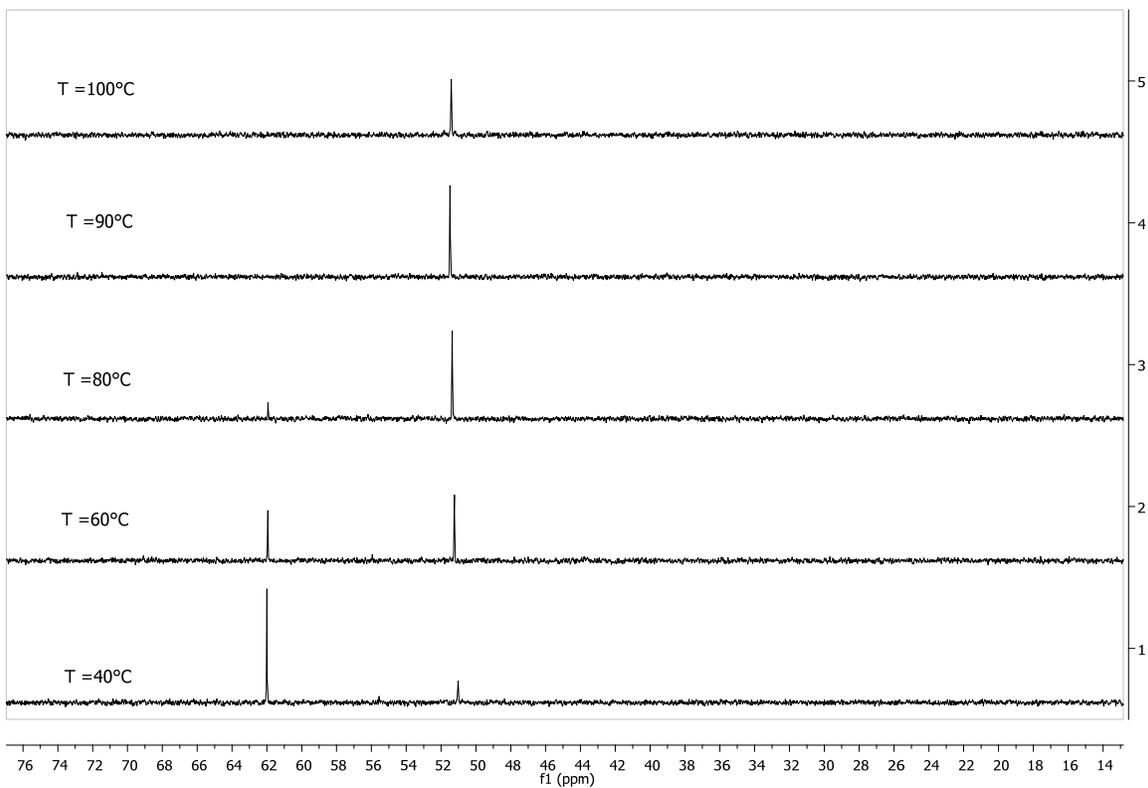
**Figure S9:** ESI-MS/MS(-) of the compound **4a** of  $m/z$  168.9, from a reaction of **4** with piperidine in PC.



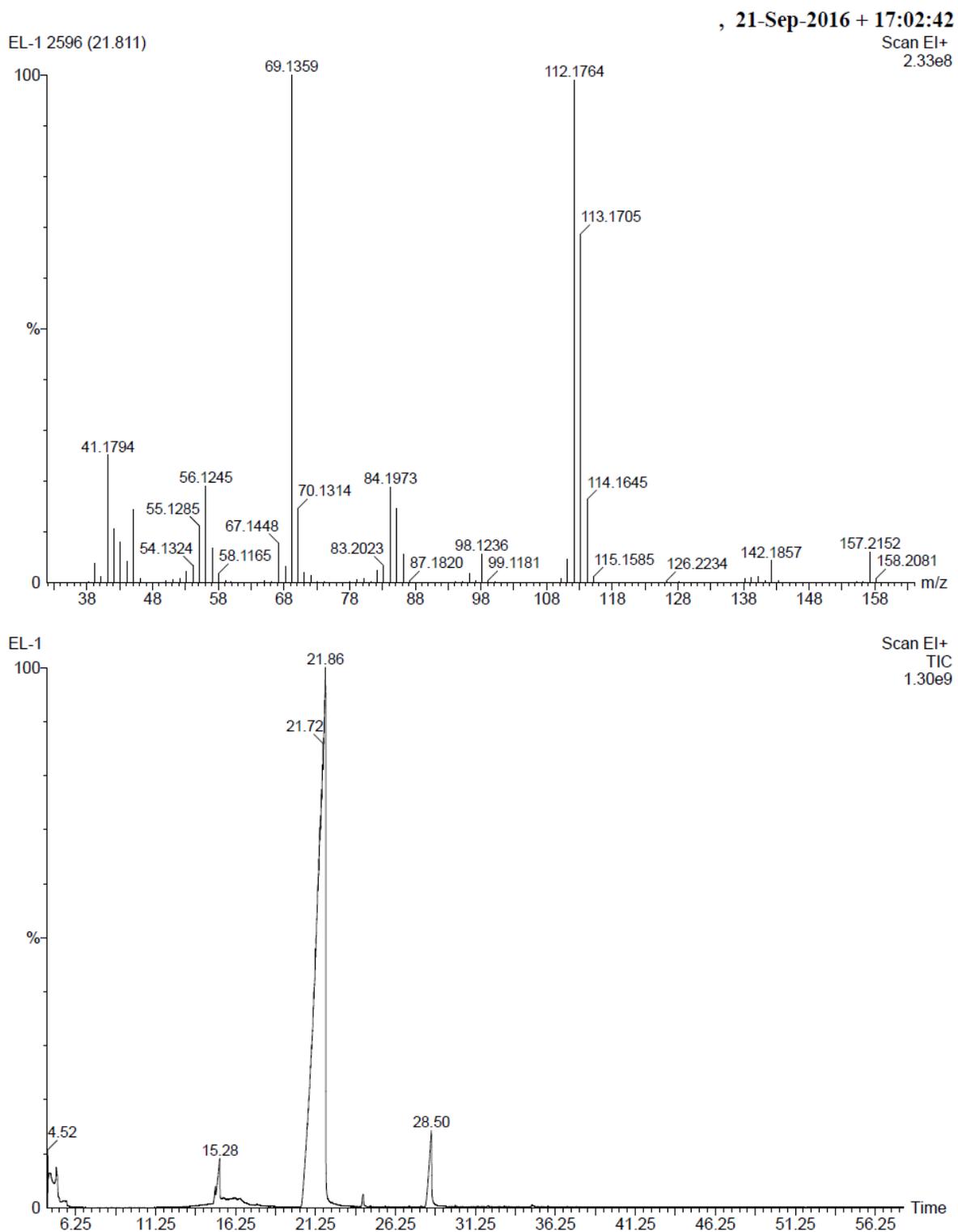
**Figure S10:** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of diazinon with piperidine in propylene carbonate at different temperatures under MW heating.



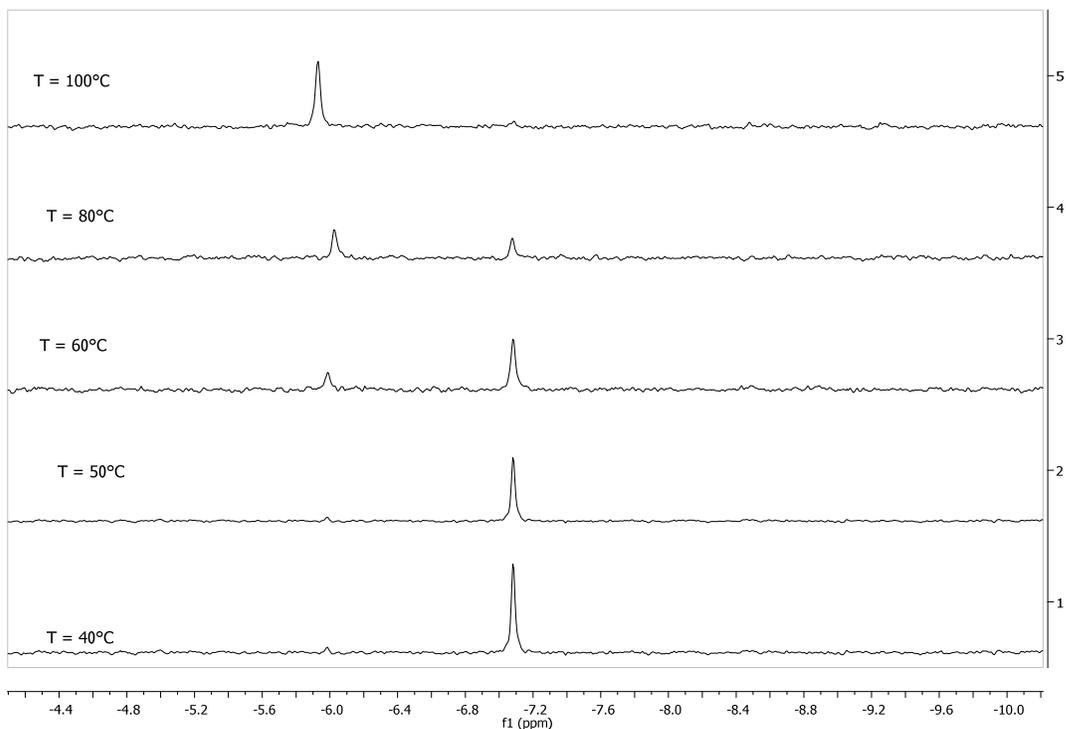
**Figure S11:** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of parathion with Bmim[ALA] in propylene carbonate at different temperatures under MW heating



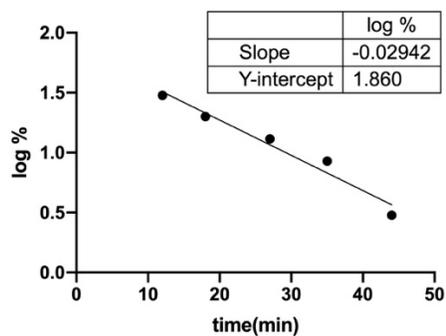
**Figure S12:** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of parathion with piperidine in propylene carbonate at different temperatures under MW heating.



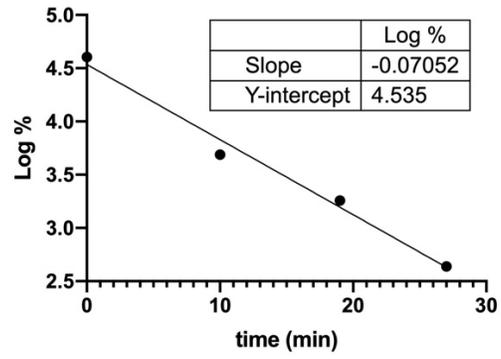
**Figure S13:** GC-MS chromatogram and mass spectrum of compound **17b** from the reaction of parathion with piperidine in PC.



**Figure S14:** Stacked  $^{31}\text{P}$ -NMR plot for the reaction of paraoxon with piperidine in propylene carbonate at different temperatures under MW heating



**Figure 15:** Plot log % vs time(min) to obtain observed first-order rate constant  $k_{\text{obs}}$  for the reaction of fenitrothion with piperidine at 25°C.



**Figure 16:** Plot log % vs time(min) to obtain observed first-order rate constant  $k_{\text{obs}}$  for the reaction of malathion with piperidine at 25°C.