

1 **Electronic Supplementary Information (ESI)**

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5 **Different molecular assemblies in two new phosphoric triamides with the**  
6 **same C(O)NHP(O)(NH)<sub>2</sub> skeleton: crystallographic study and Hirshfeld**  
7 **surface analysis**

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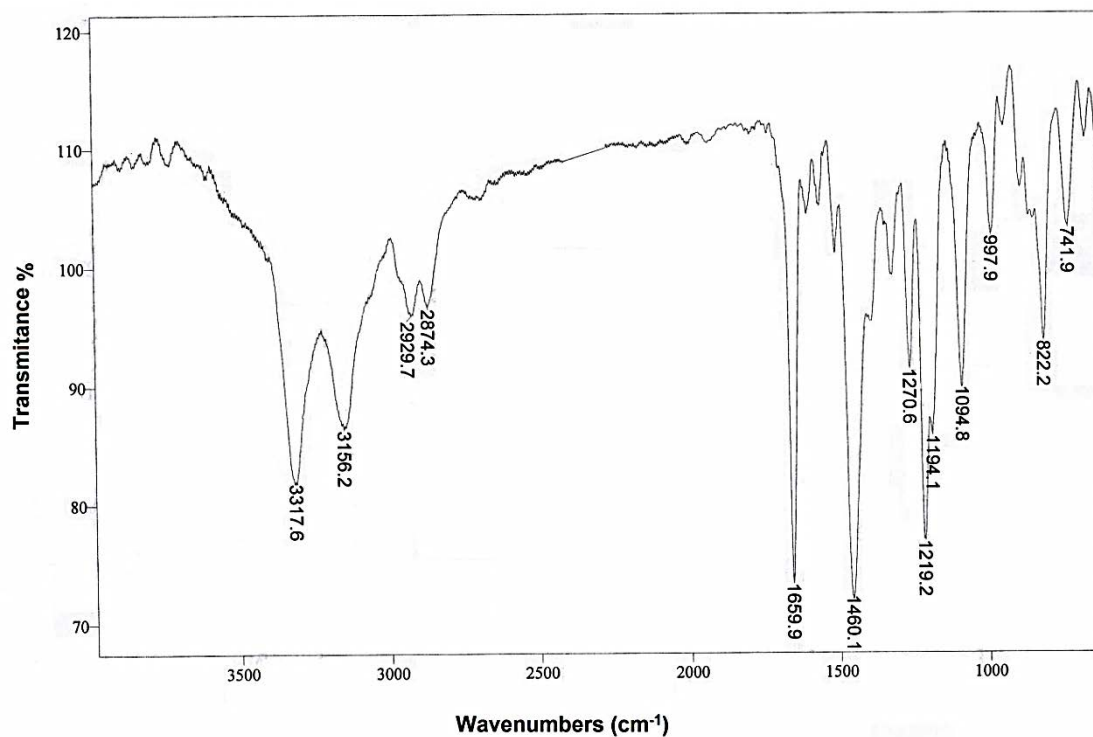
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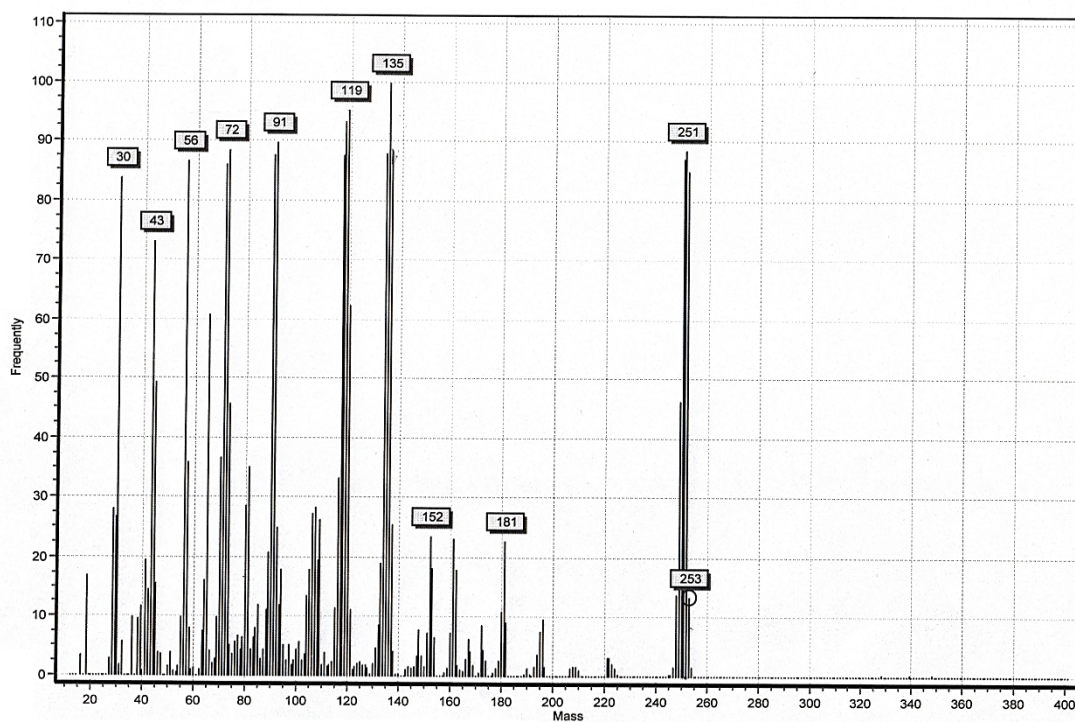
- Fig. S1.** IR spectrum of compound **1**.
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Fig. S1. IR spectrum of compound 1.

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Fig. S2. Mass spectrum of compound 1.

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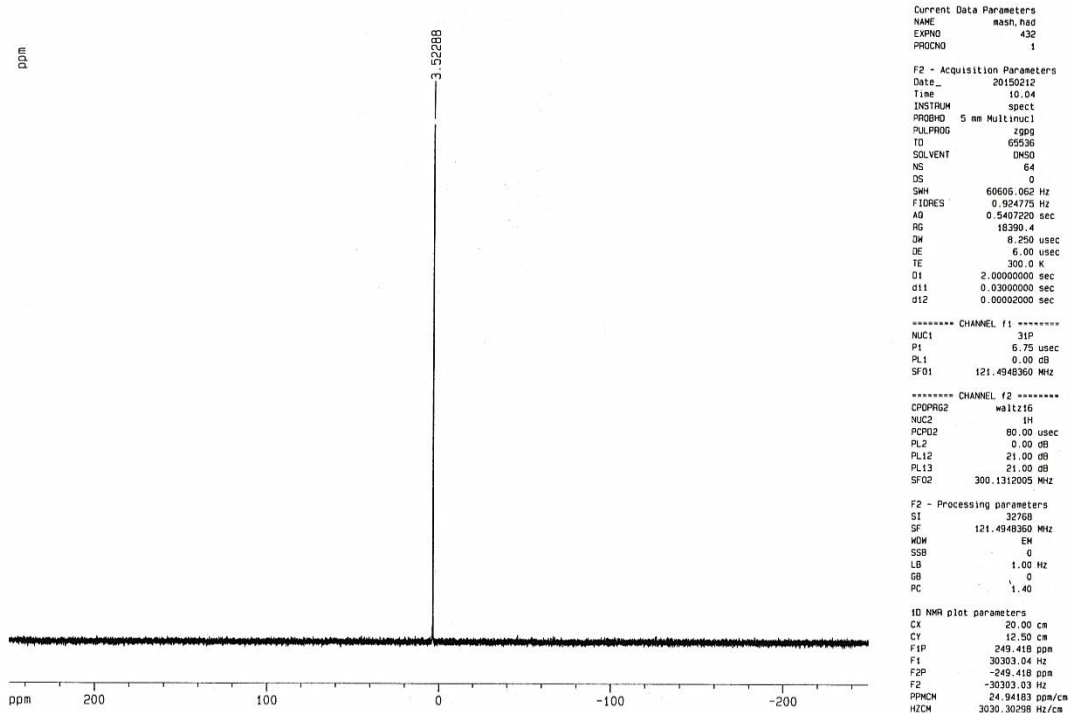


Fig. S3.  $^{31}\text{P}$  NMR spectrum of compound **1** ( $d_6$ -DMSO).

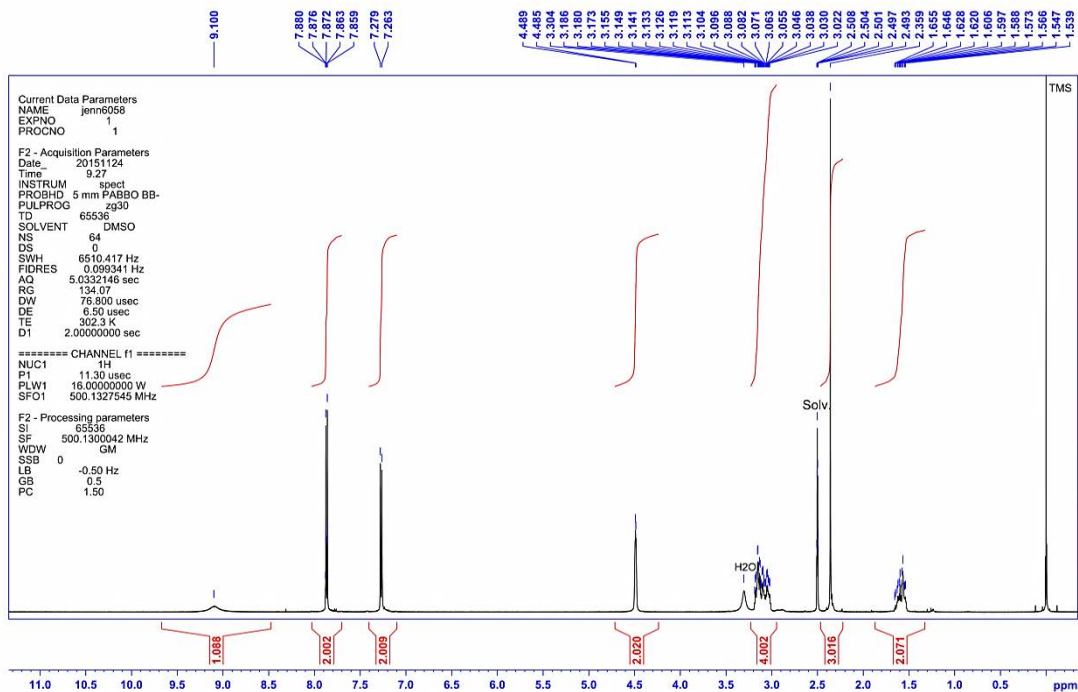
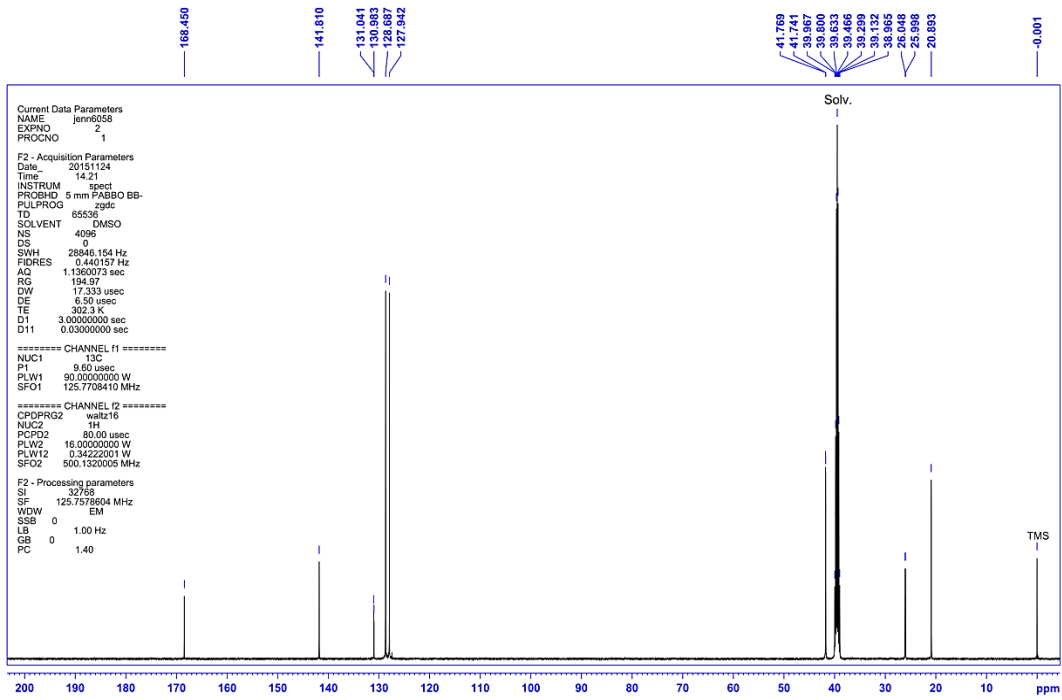


Fig. S4.  $^1\text{H}$  NMR spectrum of compound **1** ( $d_6$ -DMSO).

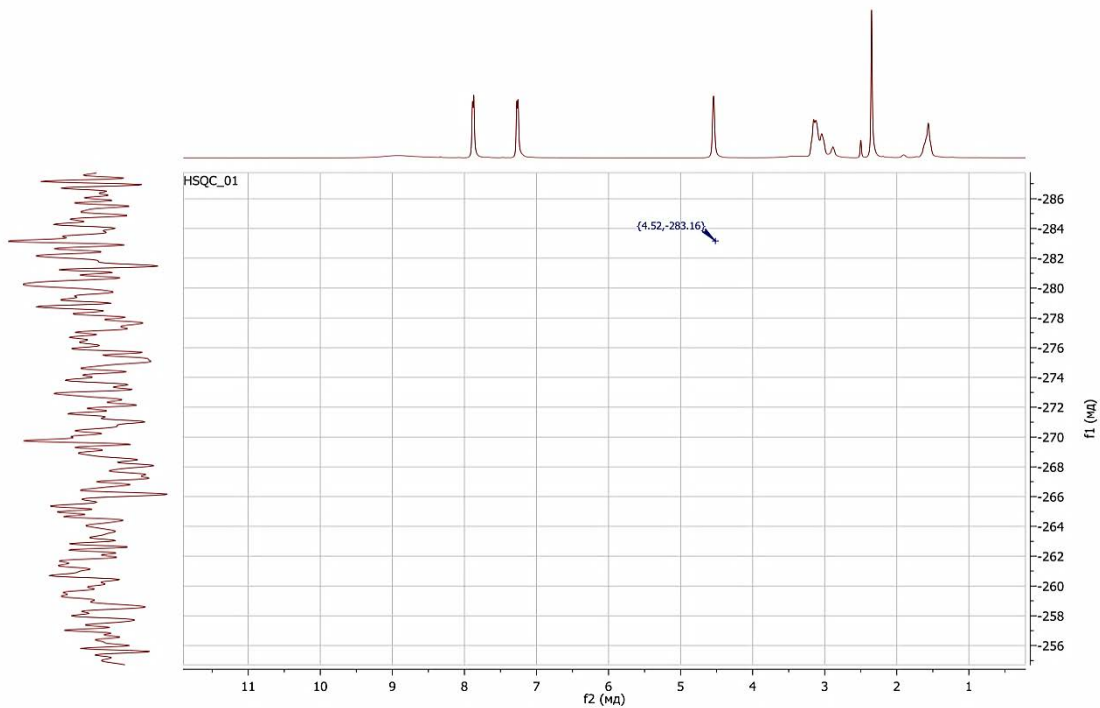


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Fig. S5.  $^{13}\text{C}$  NMR spectrum of compound **1** ( $d_6$ -DMSO).

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Fig. S6.  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound **1**.

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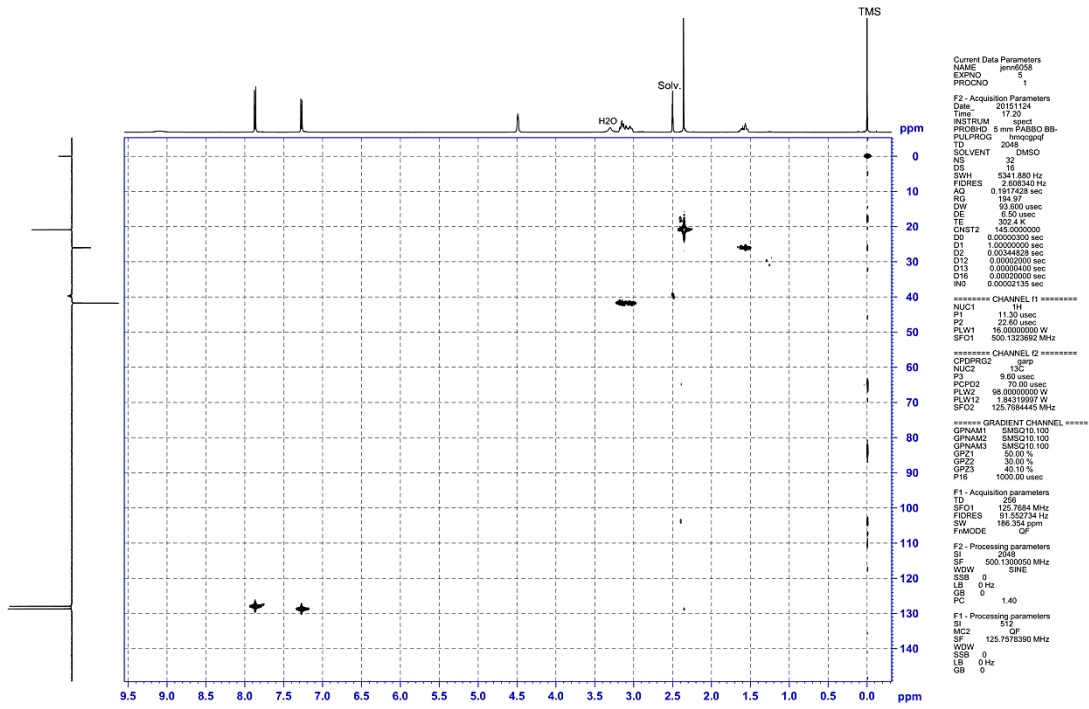


Fig. S7.  $^1\text{H}$ - $^{13}\text{C}$  HMQC spectrum of compound 1.

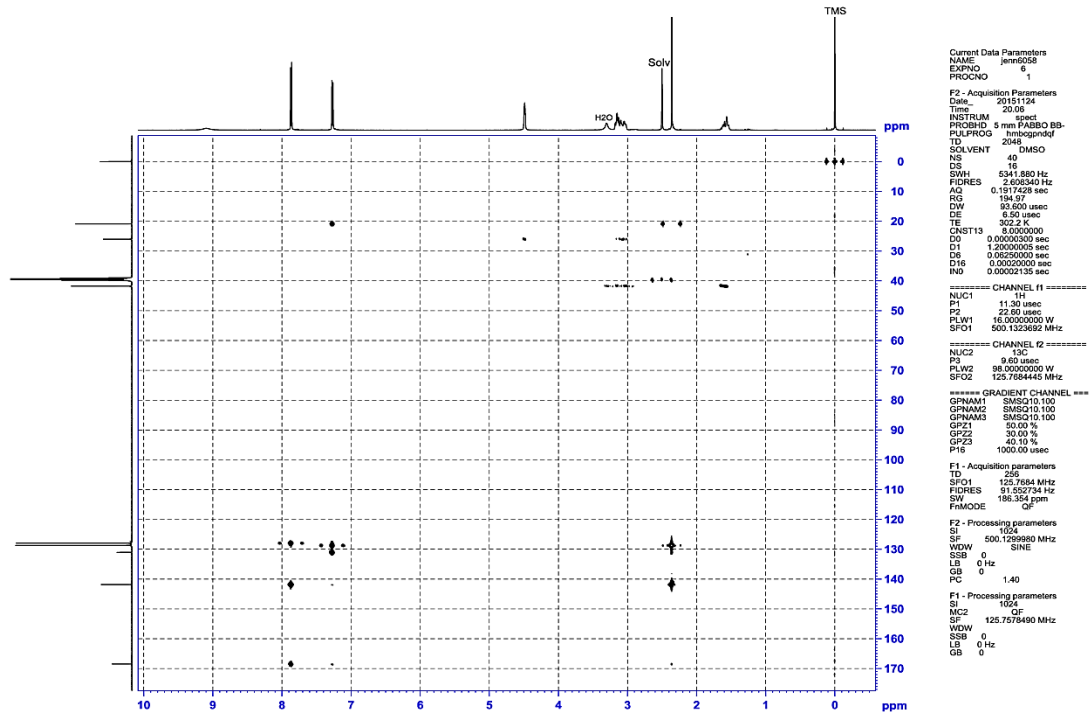
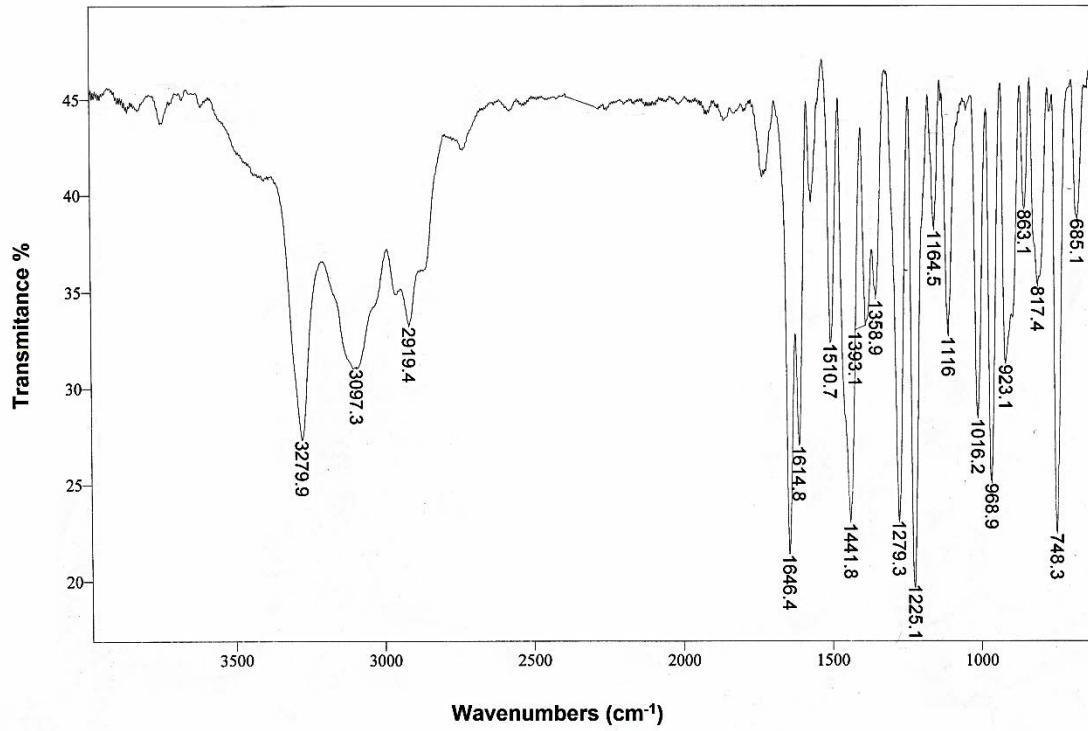


Fig. S8.  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound 1.

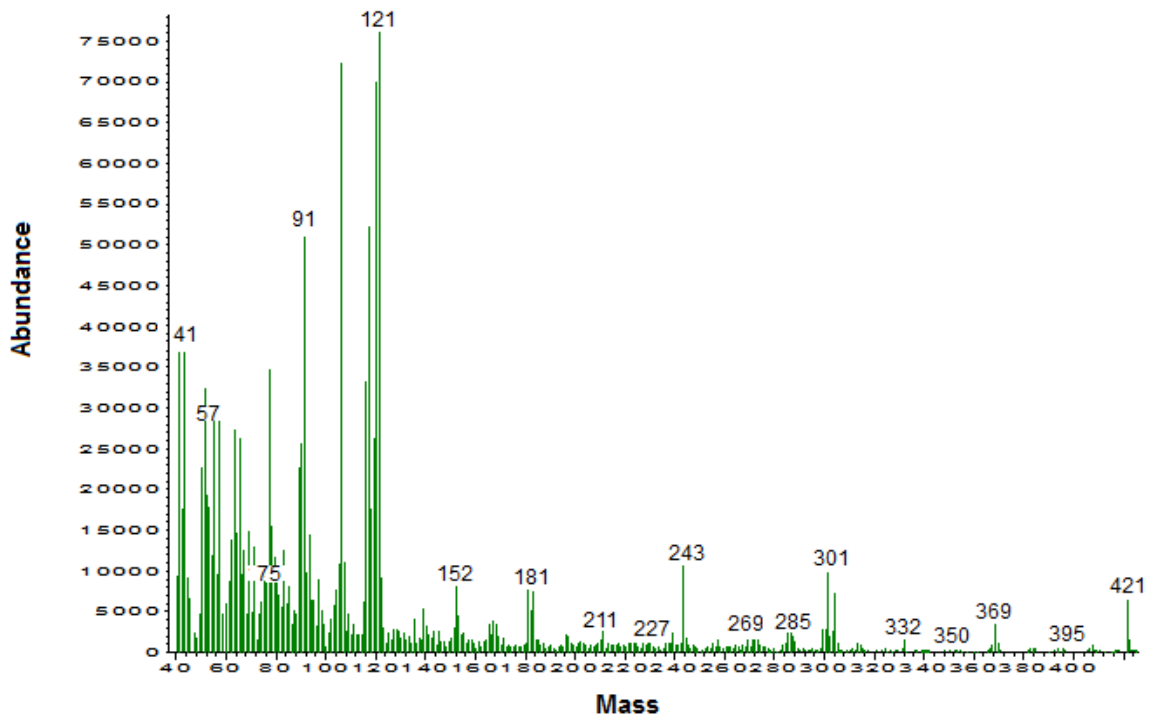


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Fig. S9. IR spectrum of compound 2.



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Fig. S10. Mass spectrum of compound 2.

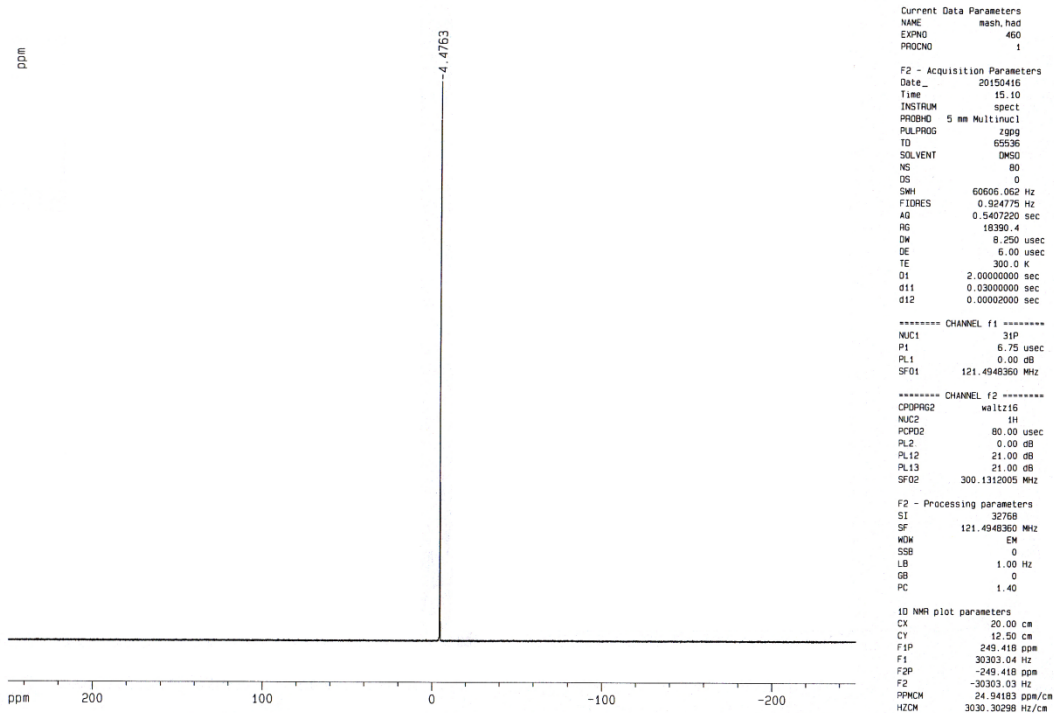


Fig. S11.  $^{31}\text{P}$  NMR spectrum of compound **2** ( $d_6$ -DMSO).

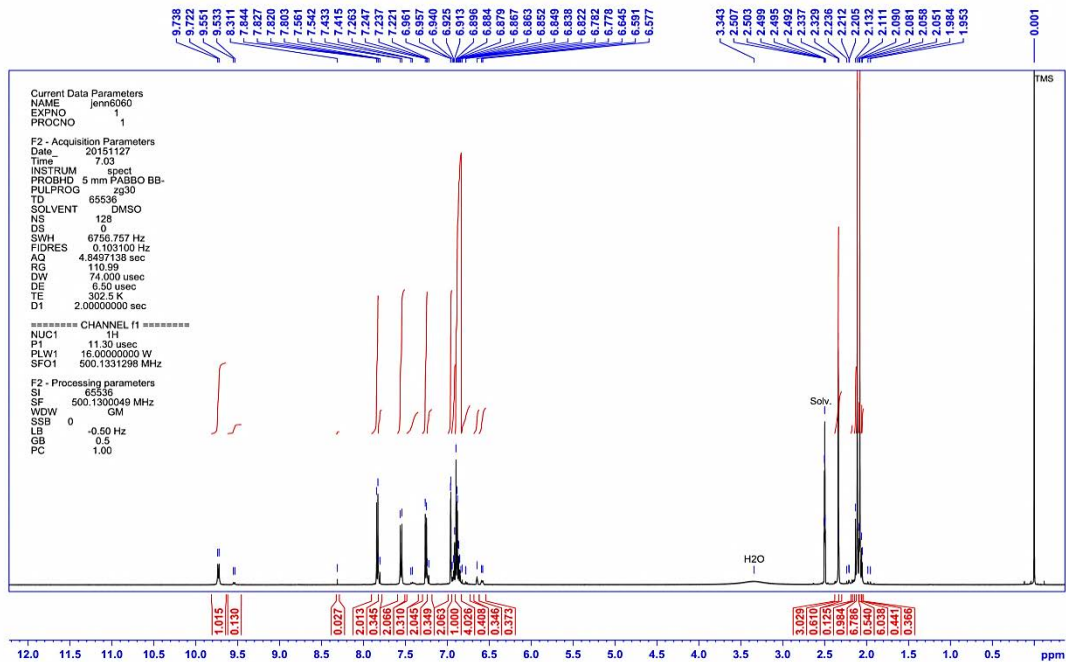
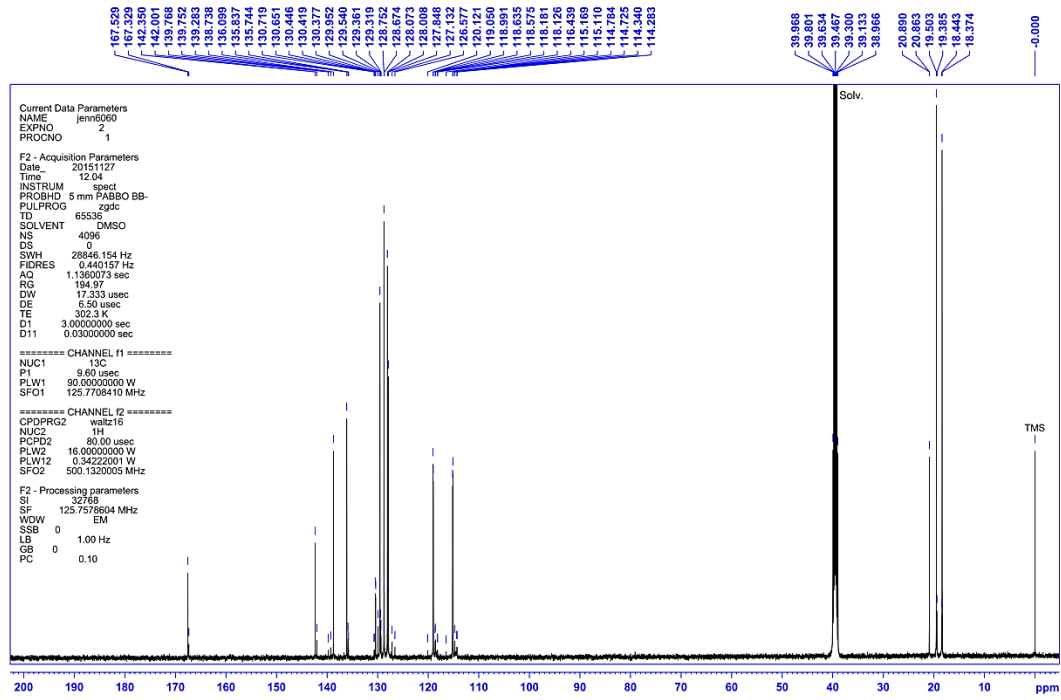


Fig. S12.  $^1\text{H}$  NMR spectrum of compound **2** ( $d_6$ -DMSO).

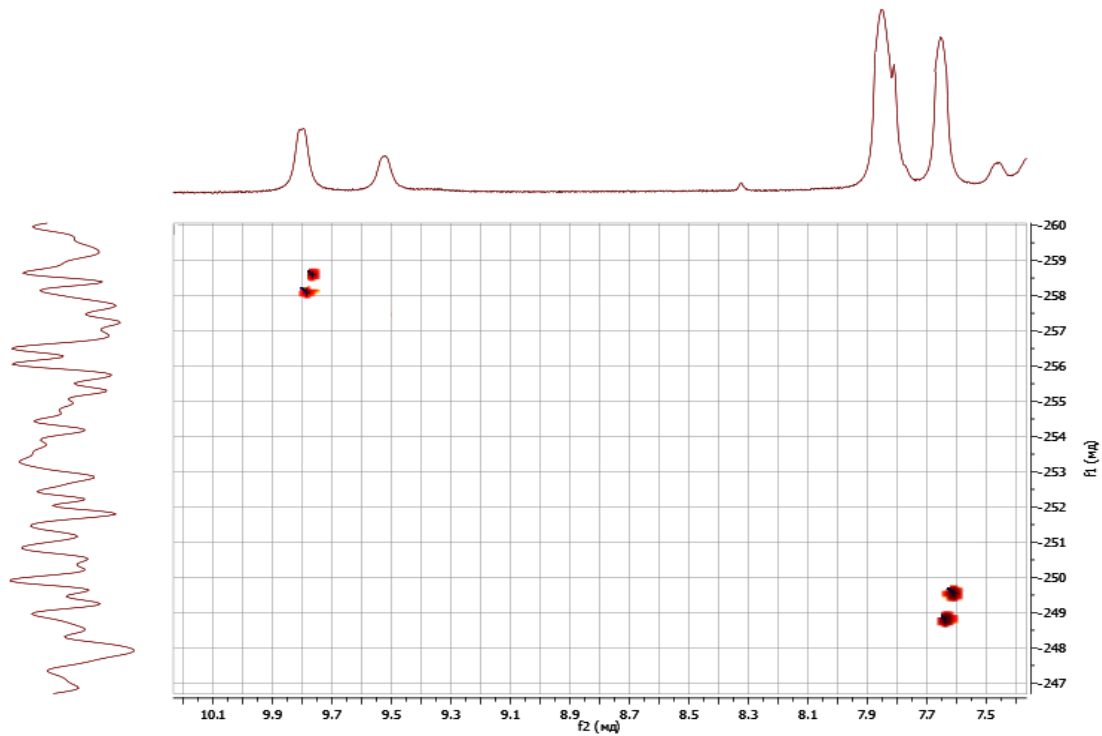




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Fig. S13.  $^{13}\text{C}$  NMR spectrum of compound 2 ( $d_6$ -DMSO).



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Fig. S14.  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectrum of compound 2.

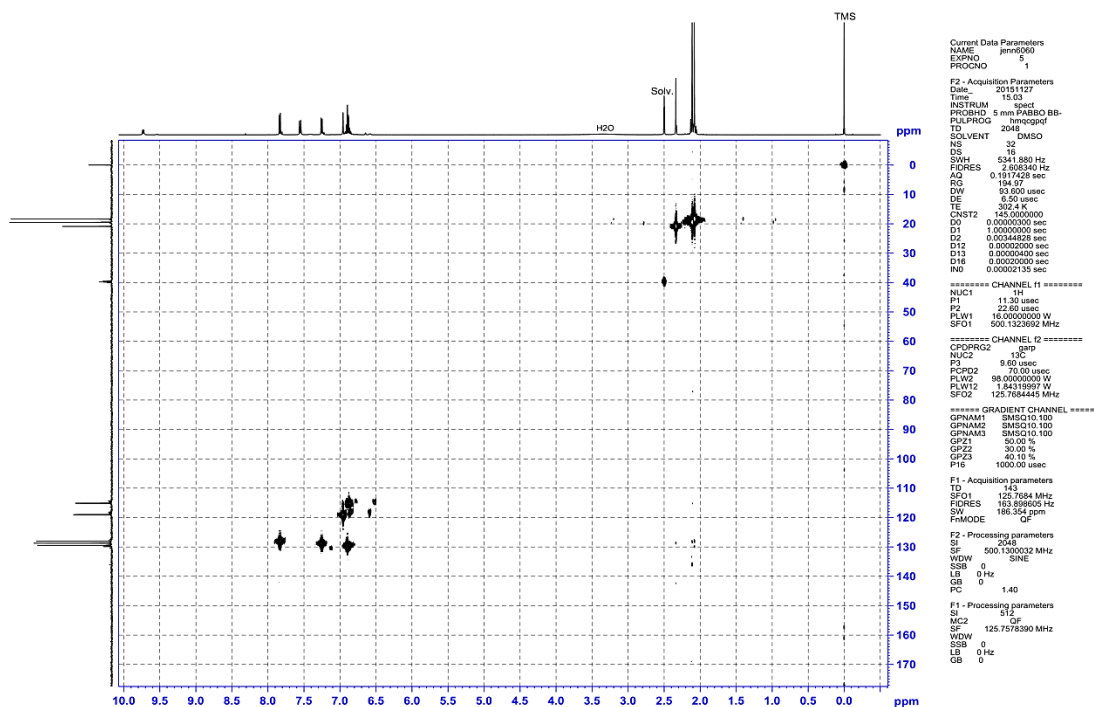


Fig. S15.  $^1\text{H}$ - $^{13}\text{C}$  HMQC spectrum of compound 2.

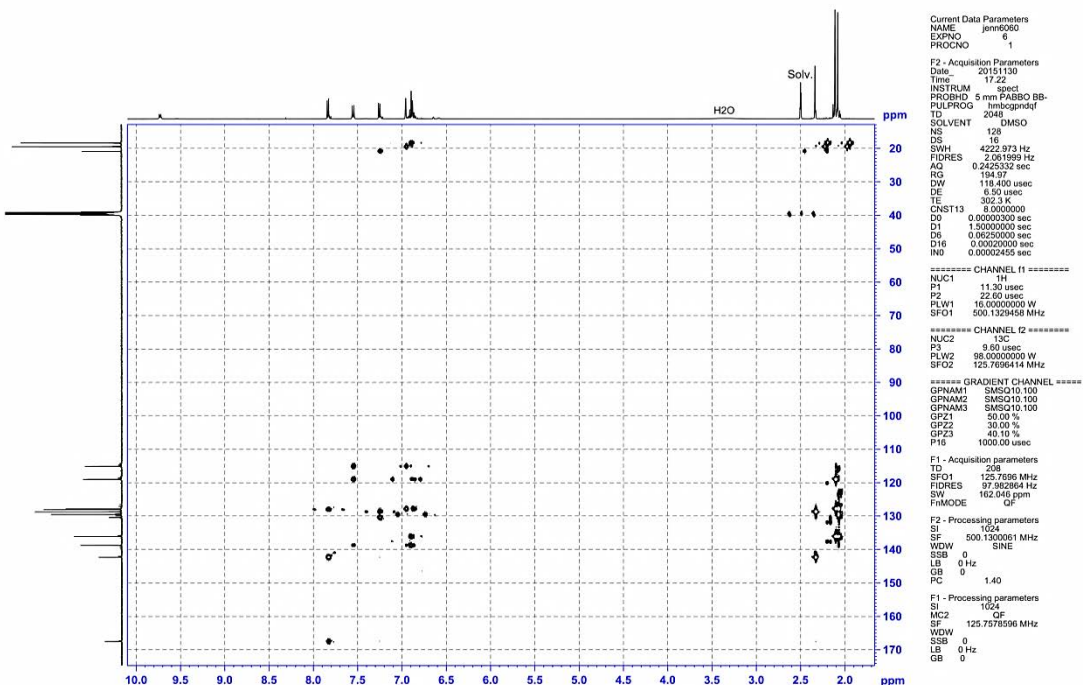


Fig. S16.  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound 2.