



## Supplementary

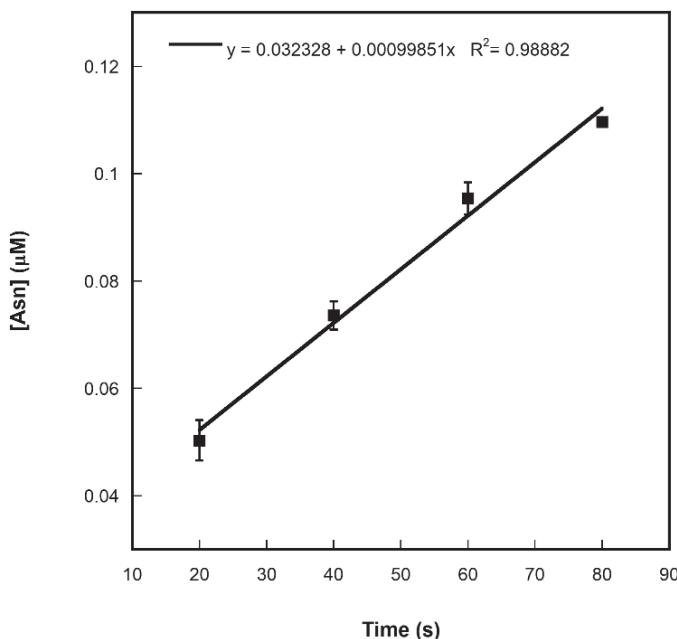
## Diethylphosphonate-containing aminoacyl-adenosine analog as inhibitor of bacterial tRNA-dependent transamidase

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Pitak Chuawong<sup>a,\*</sup>

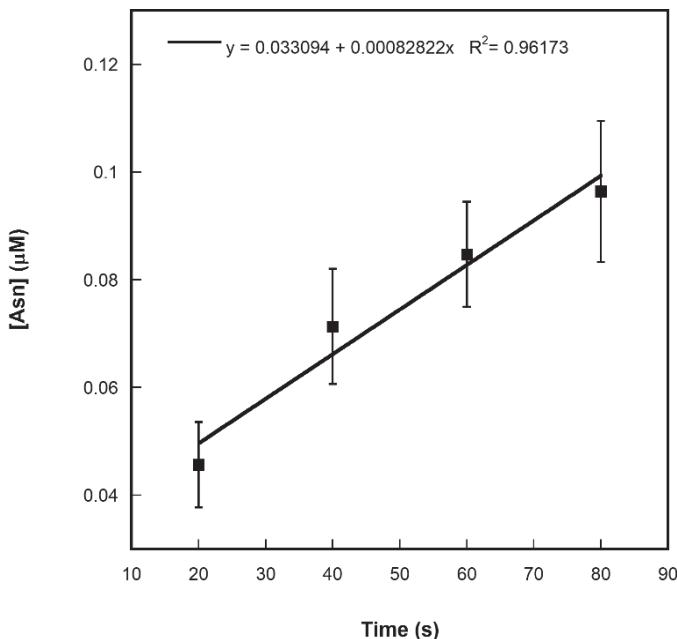
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### Supplementary Figure



**Fig. S1** Initial rate of transamidase reaction in absence of compound 1, where error bars indicate  $\pm$  SD and  $R^2$  = coefficient of determination

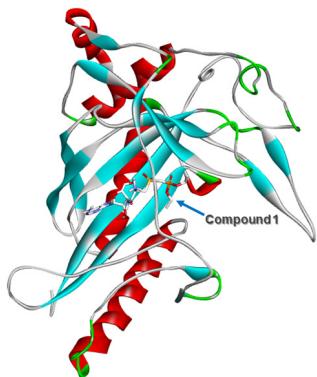


**Fig. S2** Initial rate of transamidase reaction in presence of compound 1, where error bars indicate  $\pm$  SD and  $R^2$  = coefficient of determination

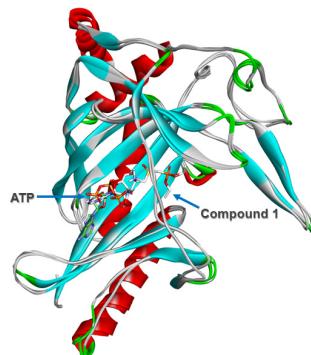
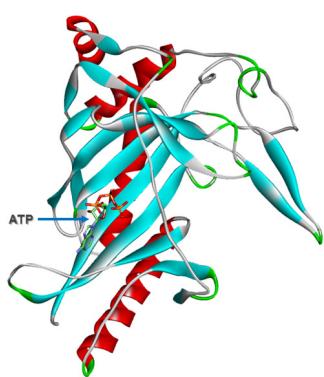
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*Helicobacter pylori* GatB active site  
(I-TASSER Model)

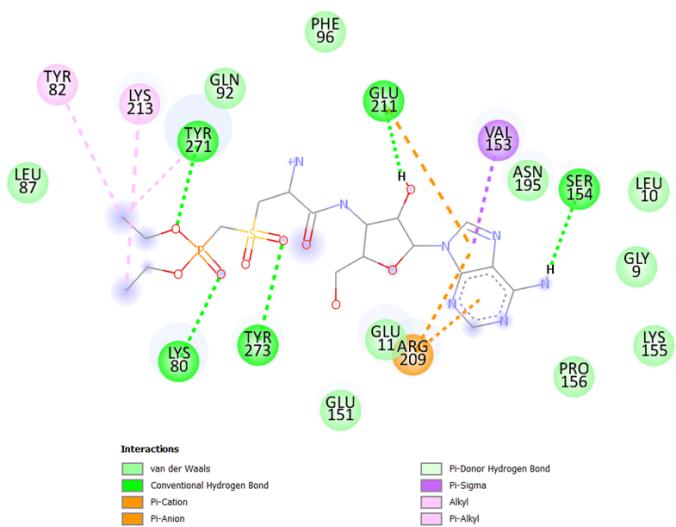


*Aquifex aeolicus* GatB active site  
(PDB ID: 3H0R)

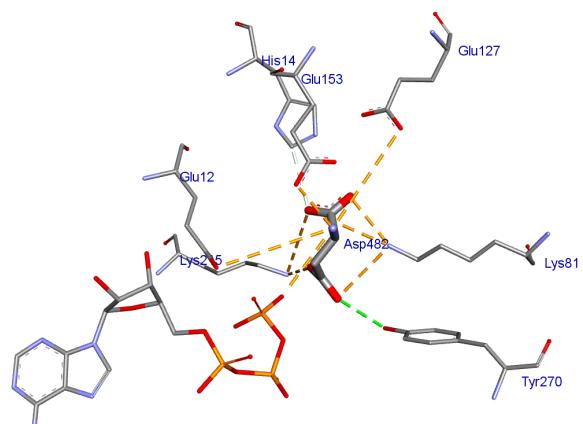


**Fig. S3** Best-docked pose of compound 1 for *H. pylori* GatB active site from molecular docking simulations (left) and crystal structure of *A. aeolicus* GatB active site co-crystallized with ATP (PDB ID: 3H0R; right), where I-TASSER = iterative threading assembly refinement and ATP = adenosine triphosphate

**Fig. S4** Superposition of *H. pylori* and *A. aeolicus* GatB active sites (structures from Fig. S3) indicating binding regions of compound 1 and adenosine triphosphate (ATP) molecule overlap at GatB active site

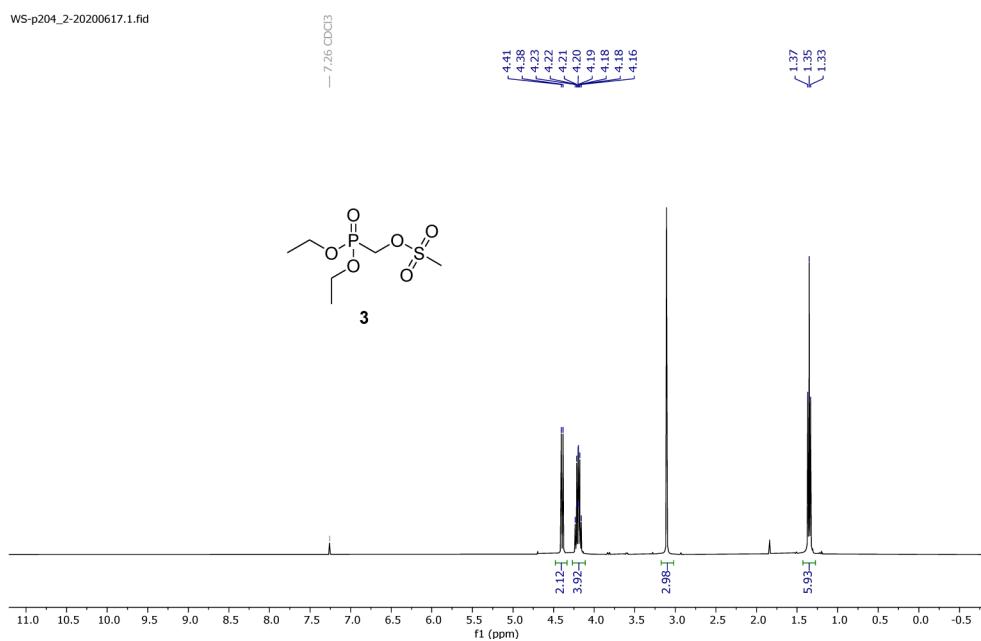


**Fig. S5** Binding interactions between compound 1 and *H. pylori* GatB active site



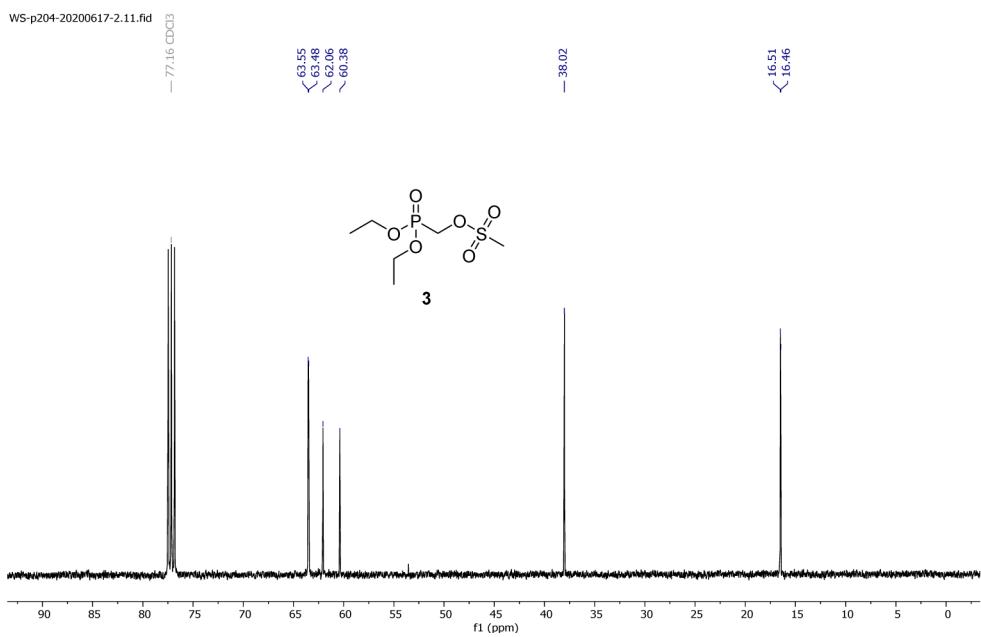
**Fig. S6** Binding interactions between aspartate and *A. aeolicus* GatB (PDB ID: 3H0R), with adenosine triphosphate (ATP) illustrated, though its interactions with GatB are omitted for clarity

WS-p204\_2-20200617.1.fid

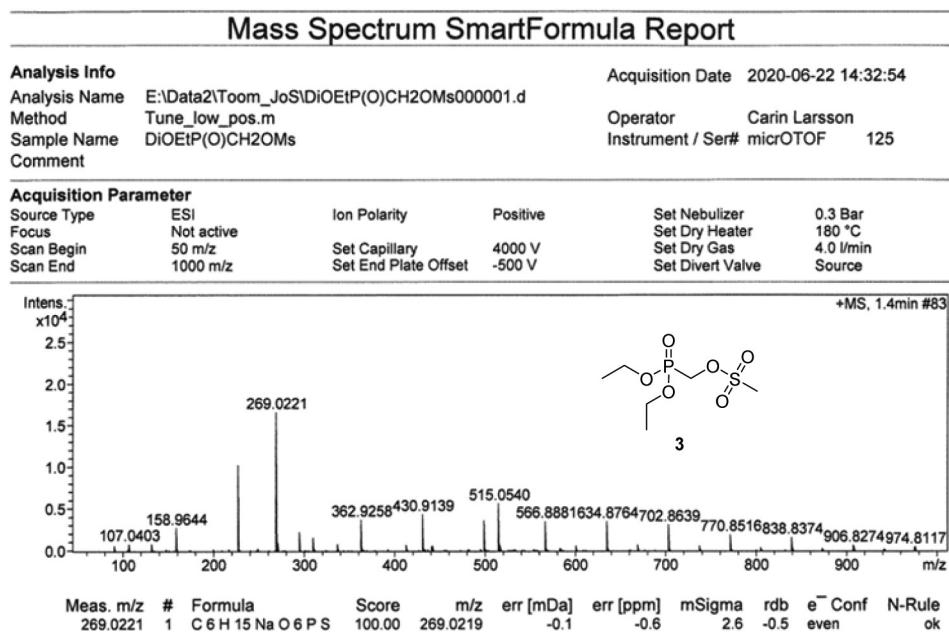


**Fig. S7** <sup>1</sup>H Nuclear magnetic resonance spectrum of compound 3 (400 MHz, CDCl<sub>3</sub>), where ppm = parts per million

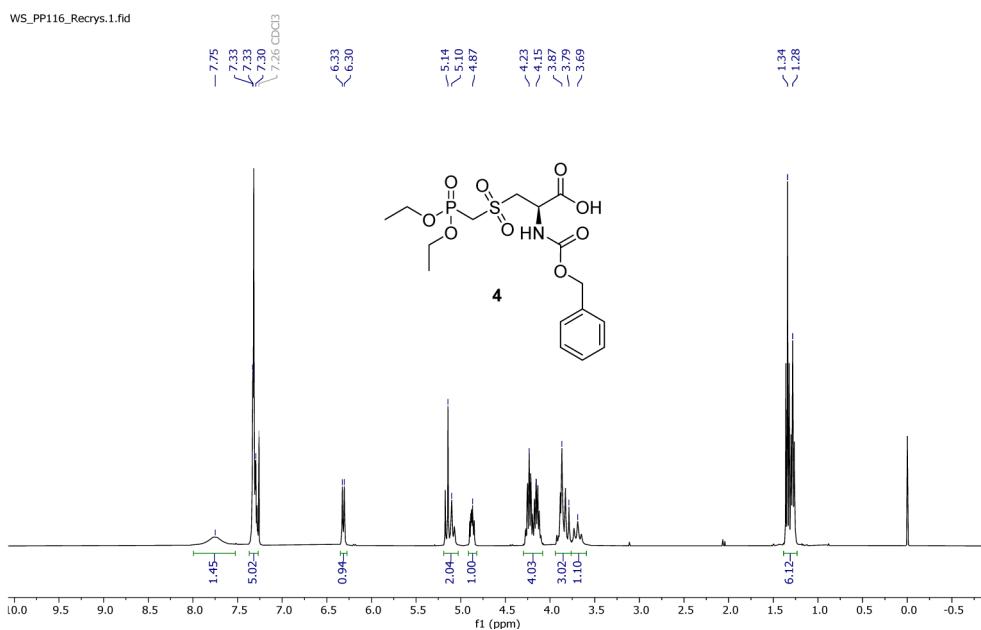
WS-p204-20200617-2.11.fid



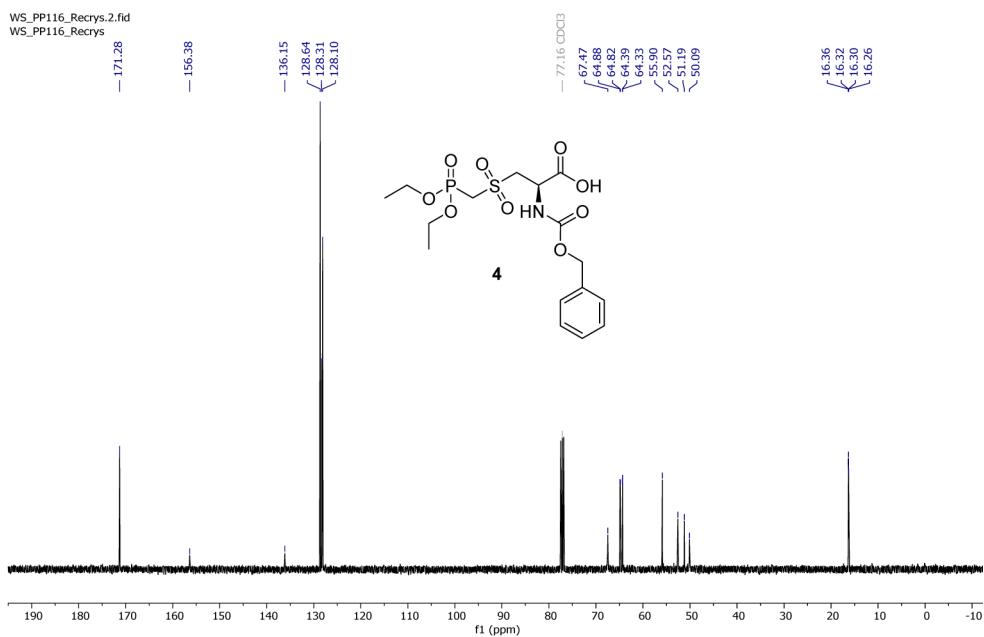
**Fig. S8** <sup>13</sup>C Nuclear magnetic resonance spectrum of compound 3 (100 MHz, CDCl<sub>3</sub>), where ppm = parts per million



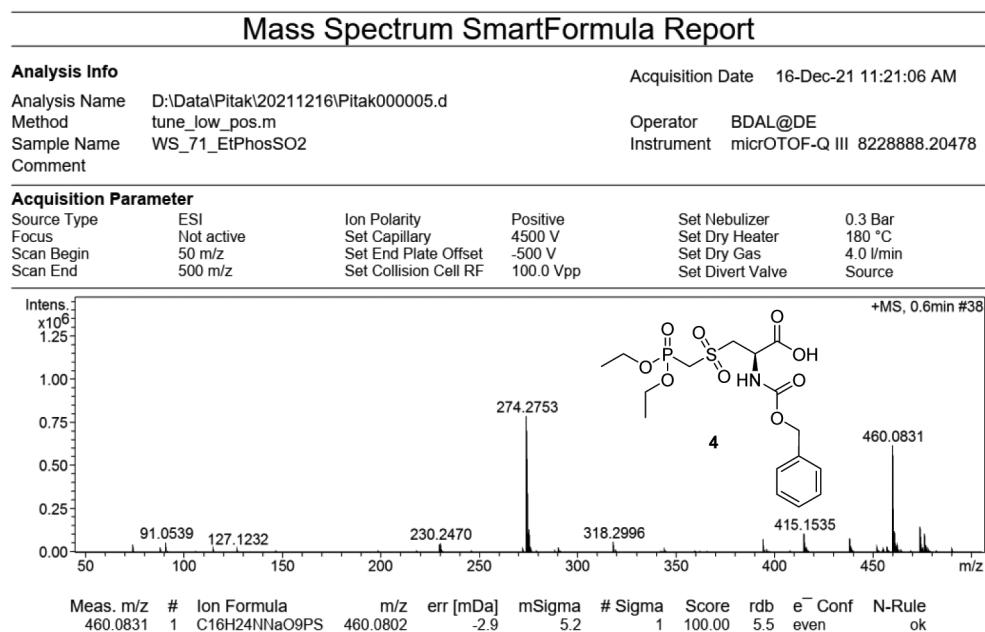
**Fig. S9** High-resolution mass spectrum (HRMS) of compound 3



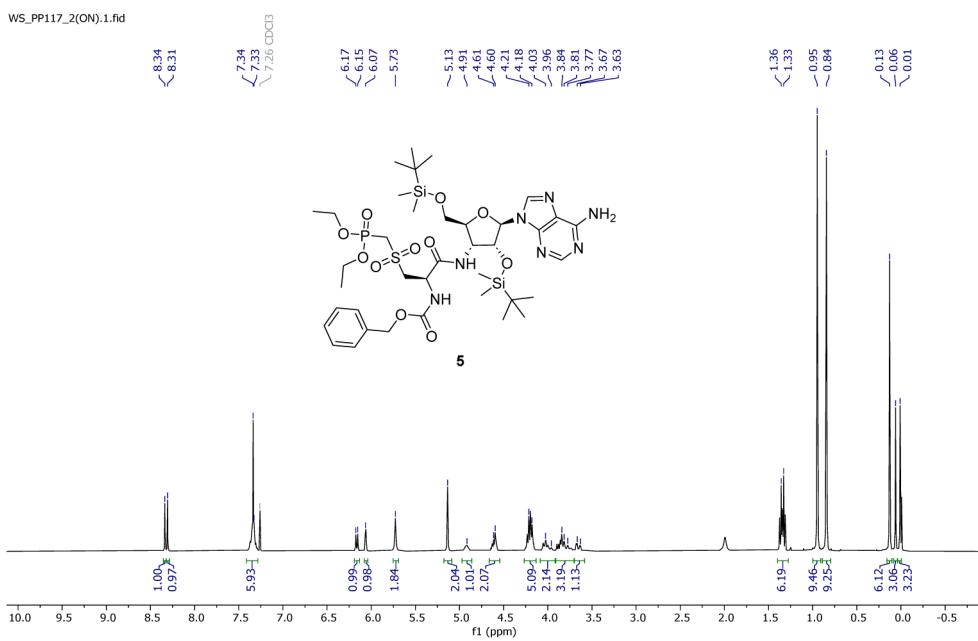
**Fig. S10** <sup>1</sup>H Nuclear magnetic resonance spectrum of compound 4 (400 MHz, CDCl<sub>3</sub>), where ppm = parts per million



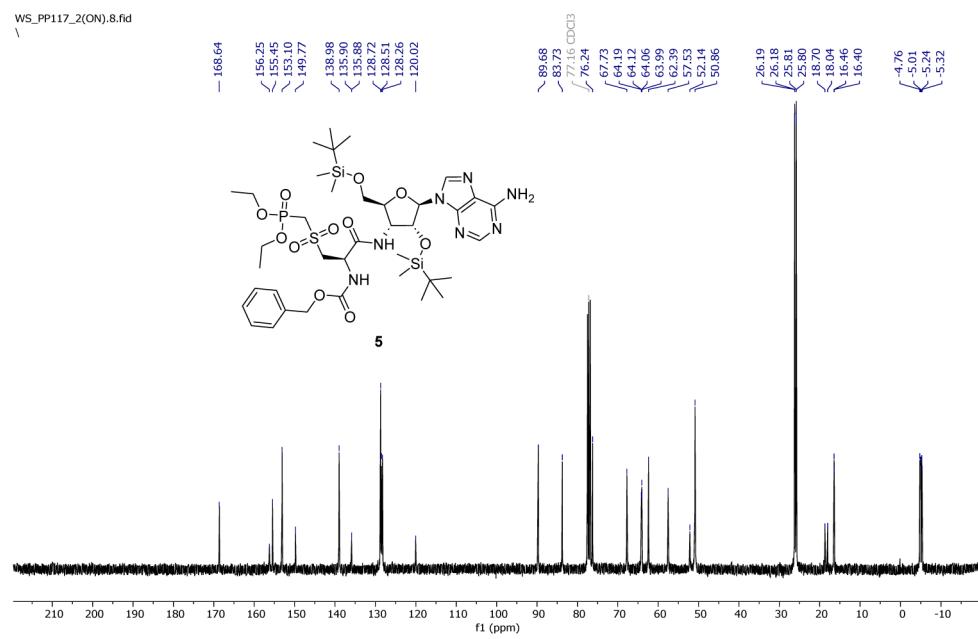
**Fig. S11**  $^{13}\text{C}$  Nuclear magnetic resonance spectrum of compound 4 (100 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



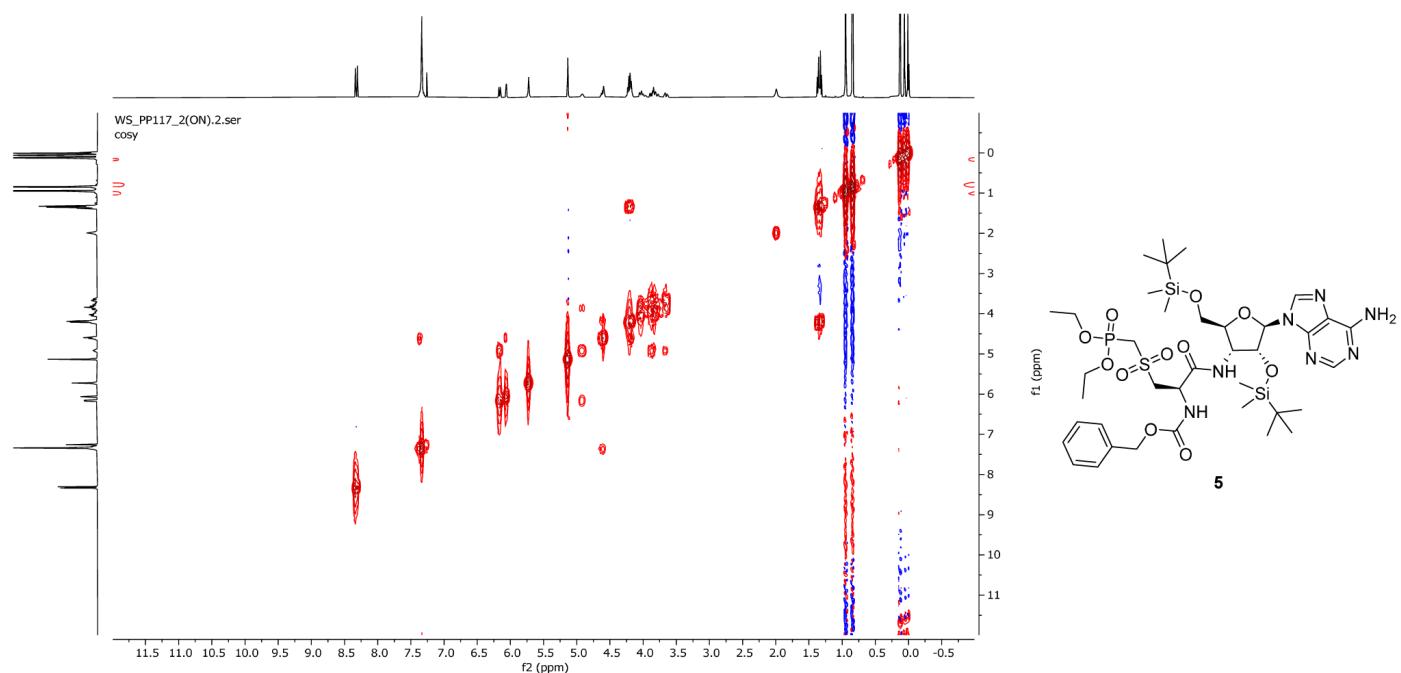
**Fig. S12** High-resolution mass spectrum (HRMS) of compound 4



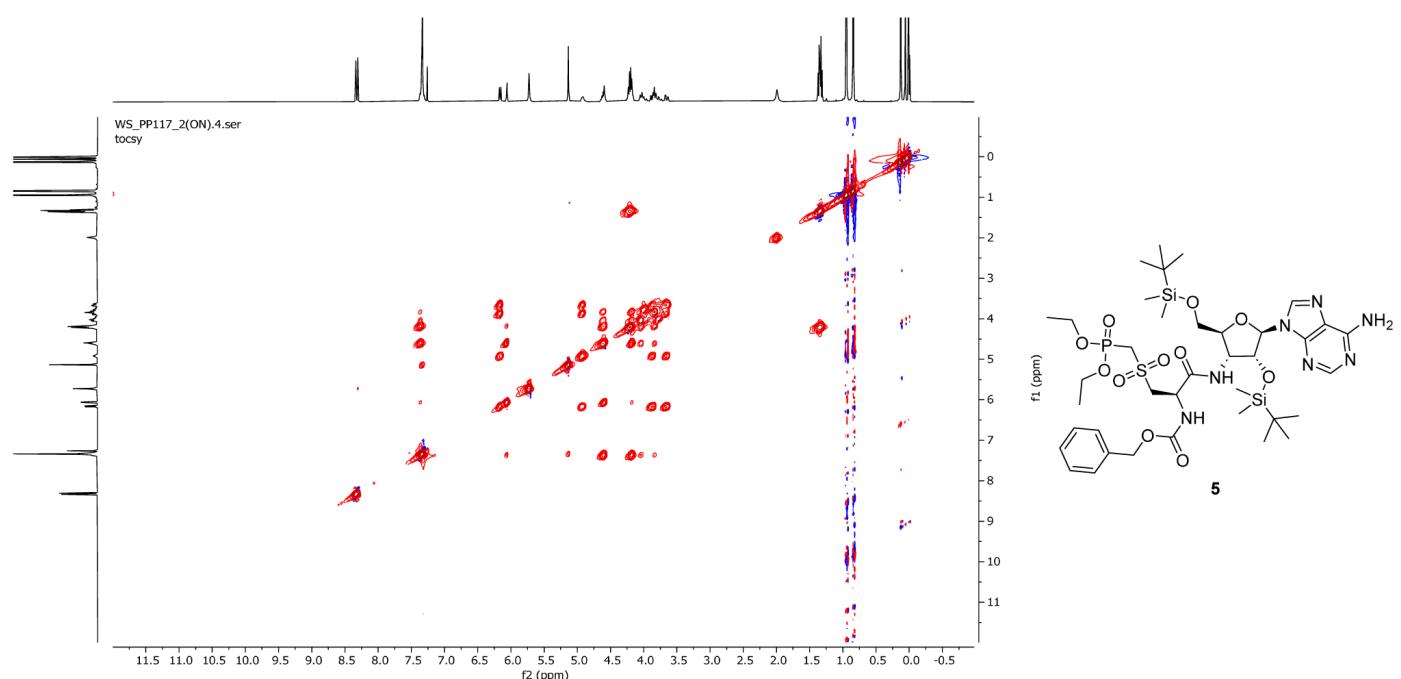
**Fig. S13**  $^1\text{H}$  Nuclear magnetic resonance spectrum of compound 5 (400 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



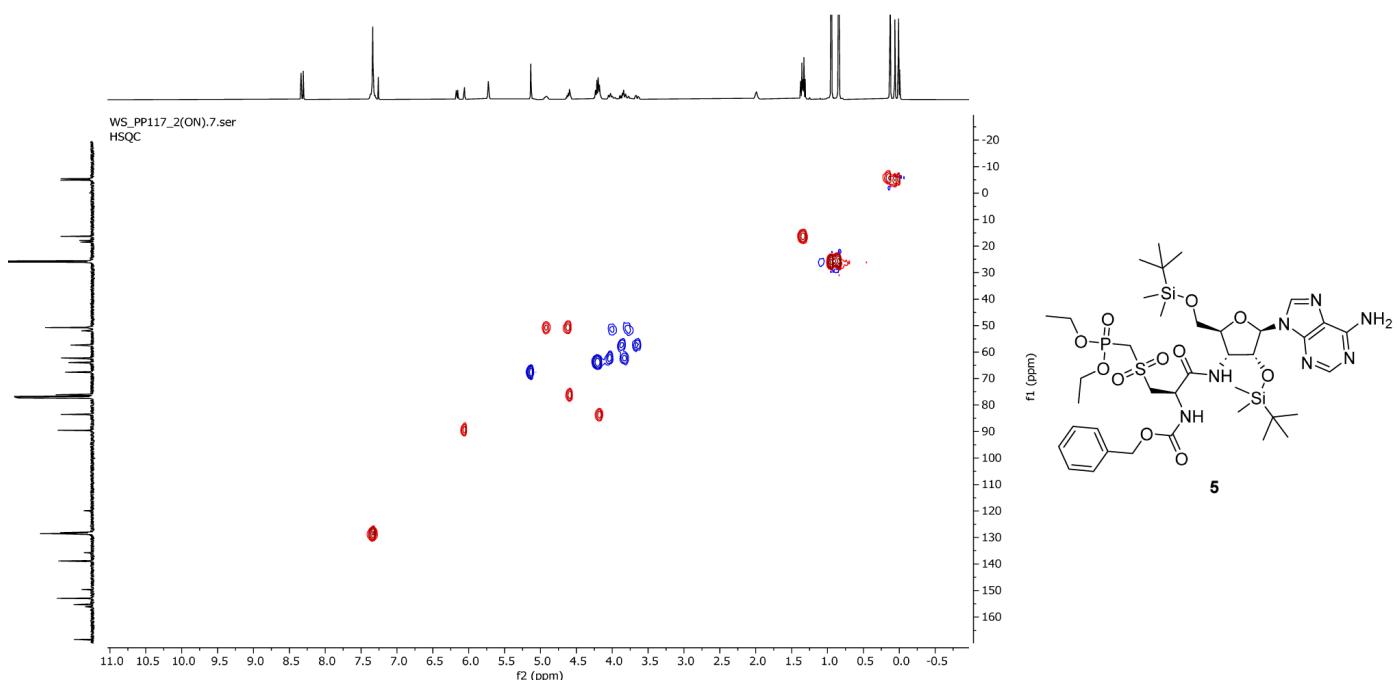
**Fig. S14**  $^{13}\text{C}$  Nuclear magnetic resonance spectrum of compound 5 (100 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



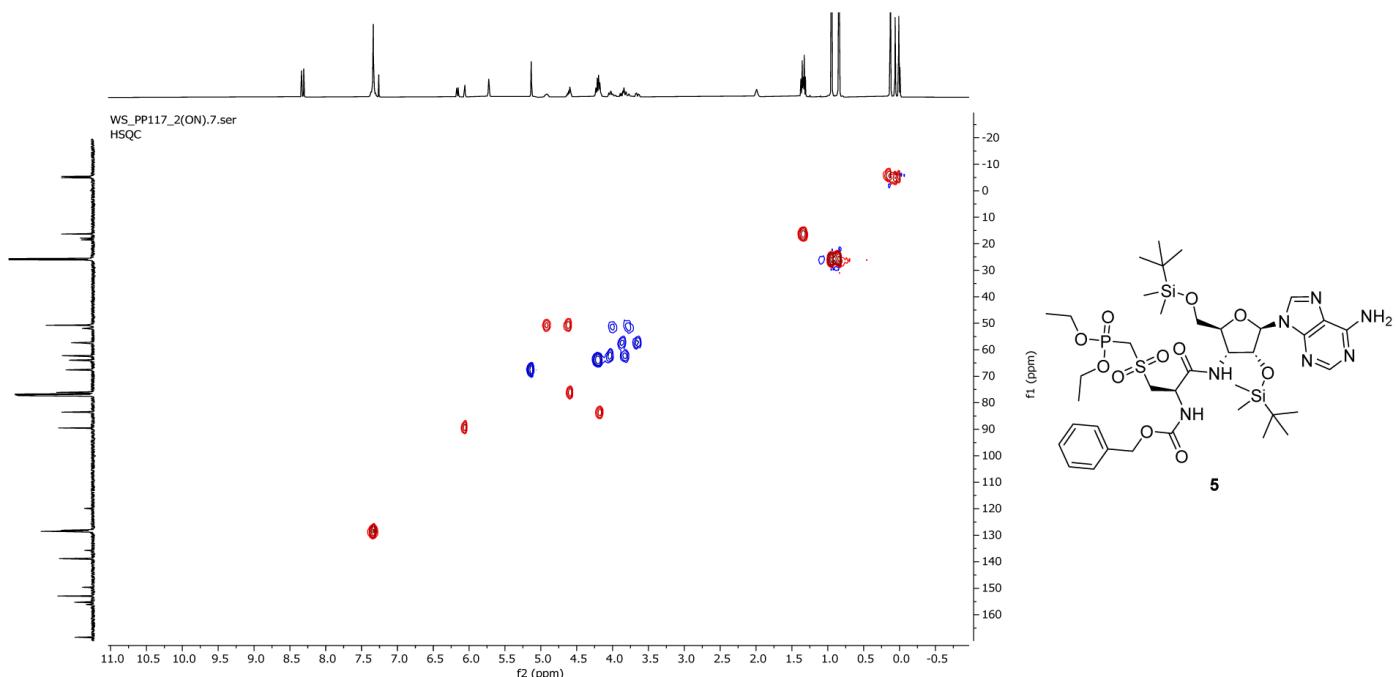
**Fig. S15** Correlated spectrum of compound 5 (400 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



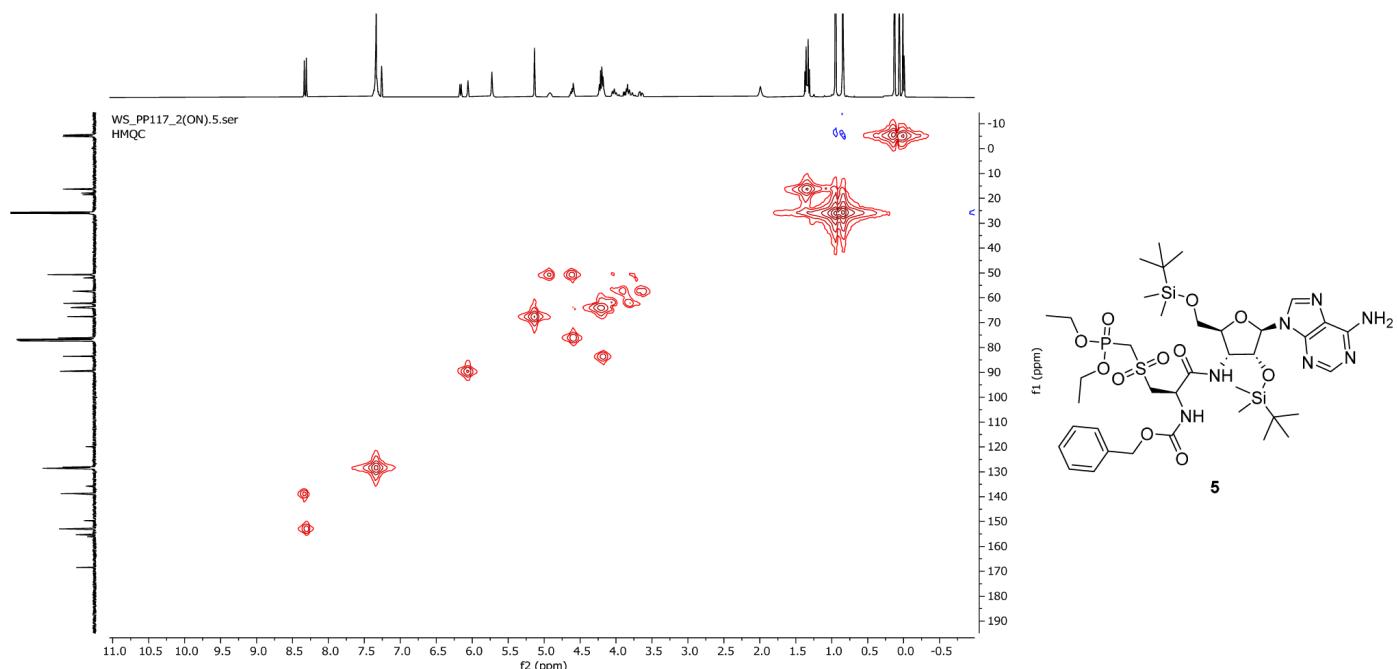
**Fig. S16** Total correlation spectrum of compound 5 (400 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



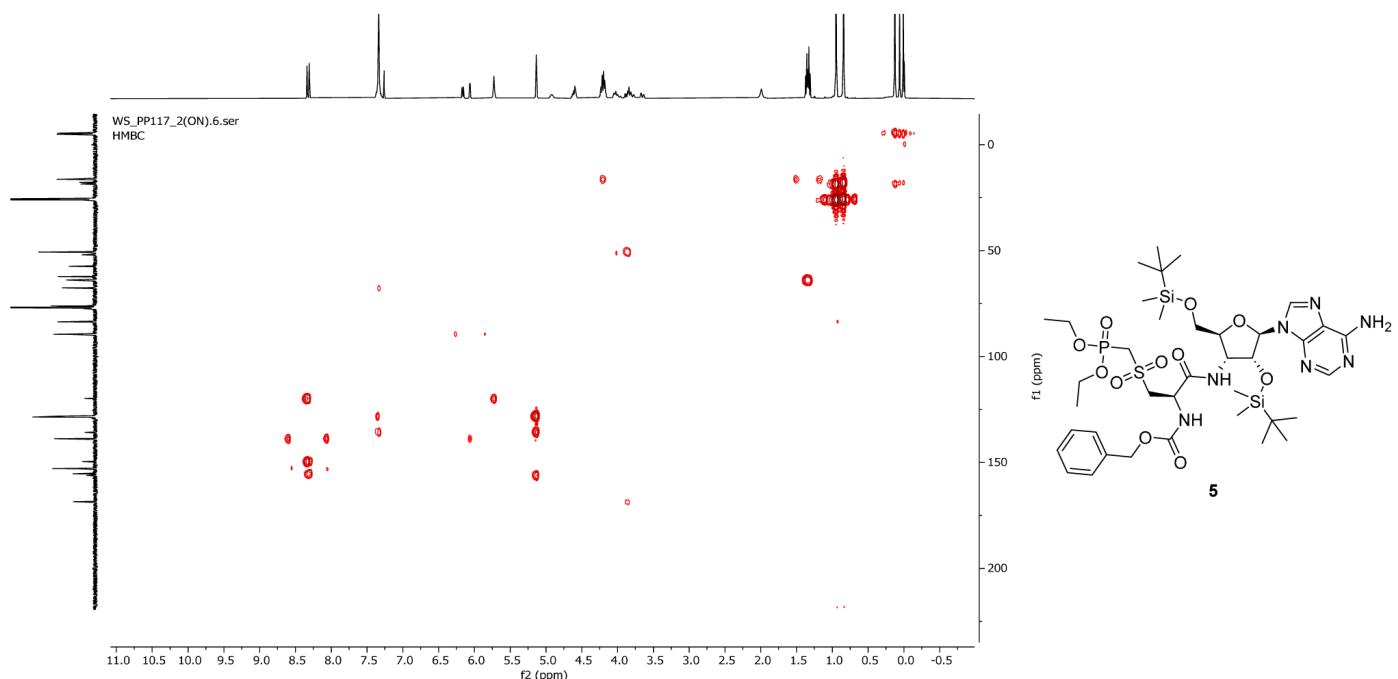
**Fig. S17** Nuclear Overhauser effect spectrum of compound 5 (400 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



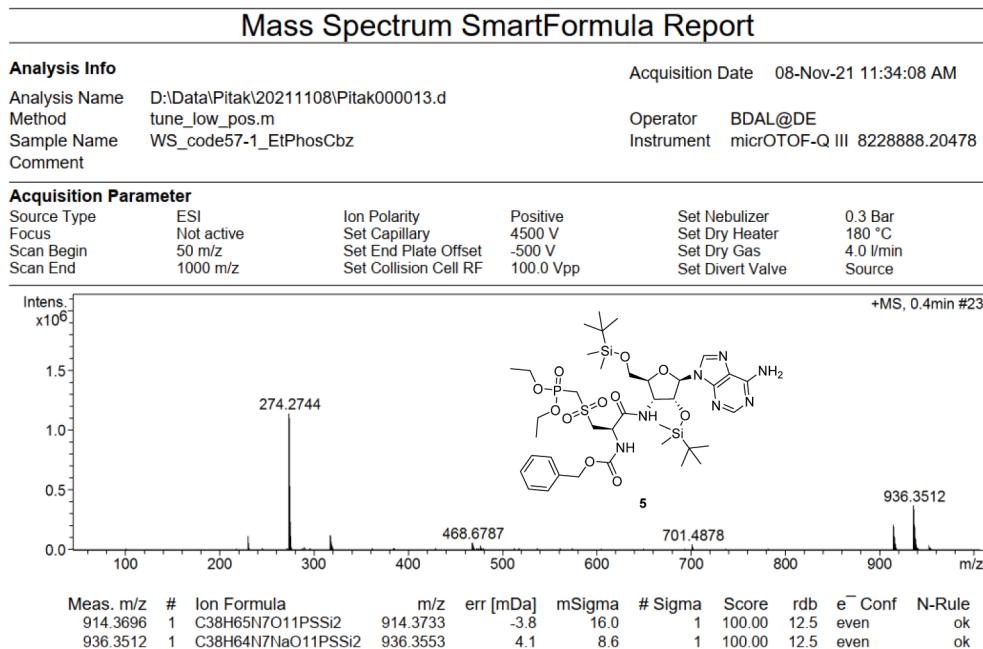
**Fig. S18** HSQC-edited spectrum of compound 5 (400 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



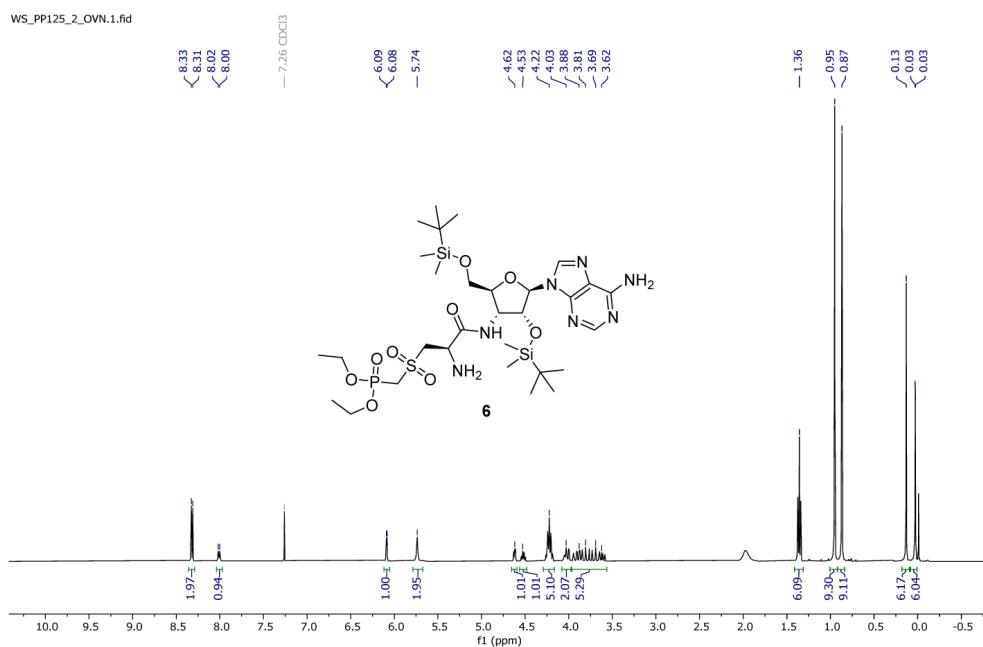
**Fig. S19** HMQC spectrum of compound 5 (400 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



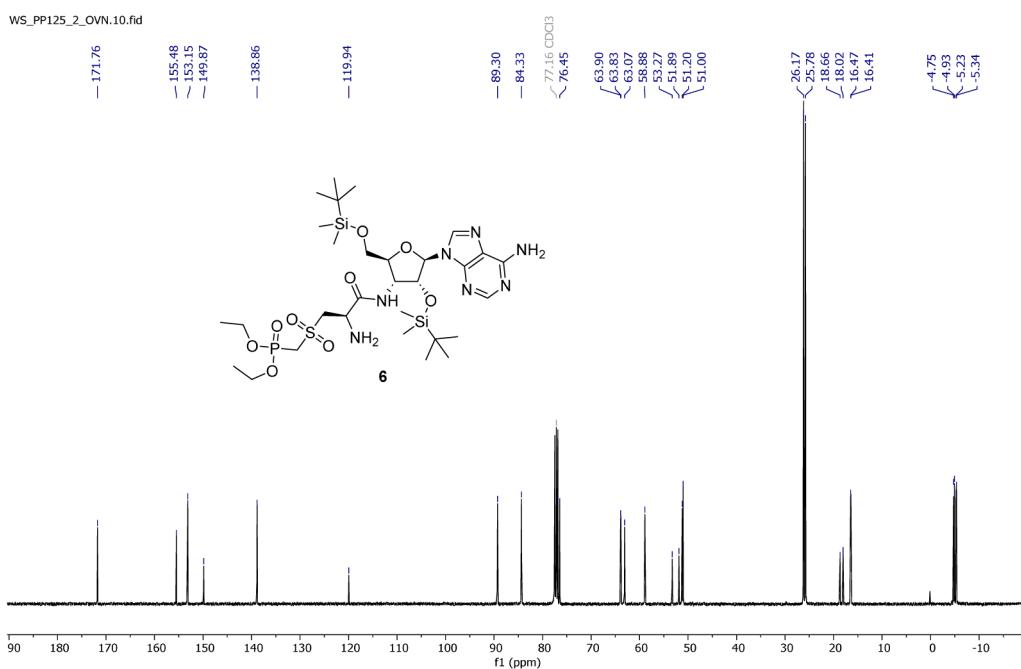
**Fig. S20** HMBC spectrum of compound 5 (400 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



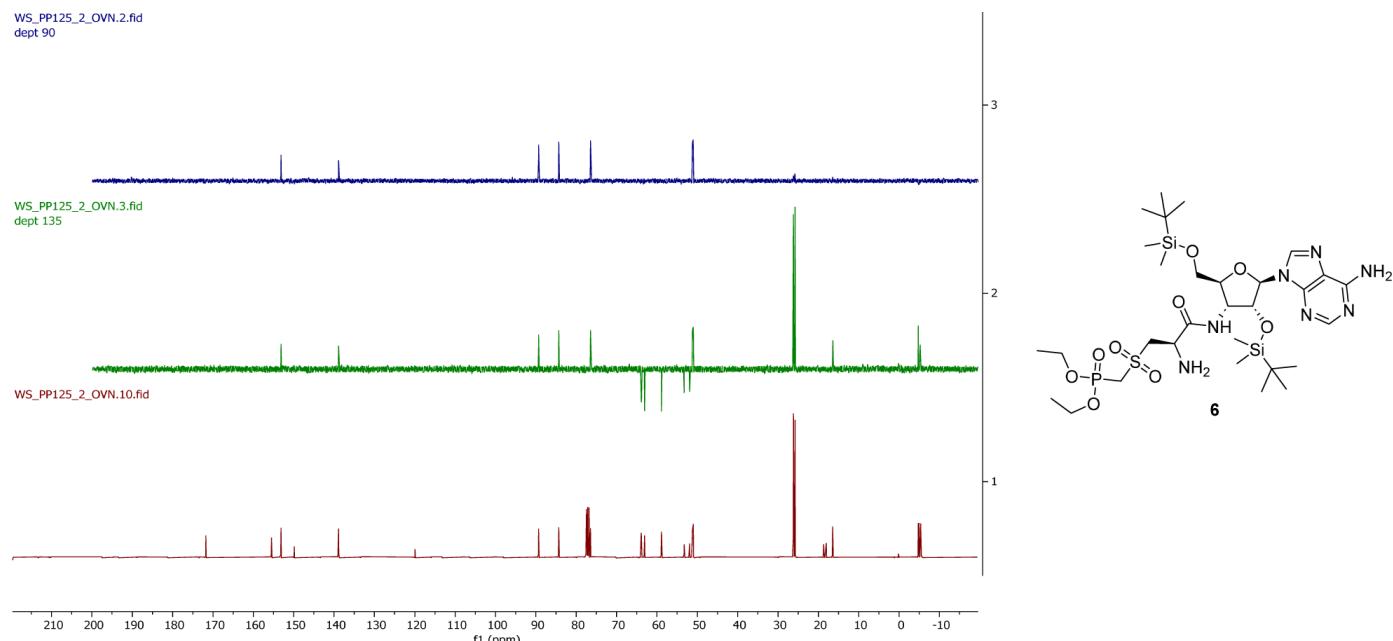
**Fig. S21** High-resolution mass spectrum (HRMS) of compound 5



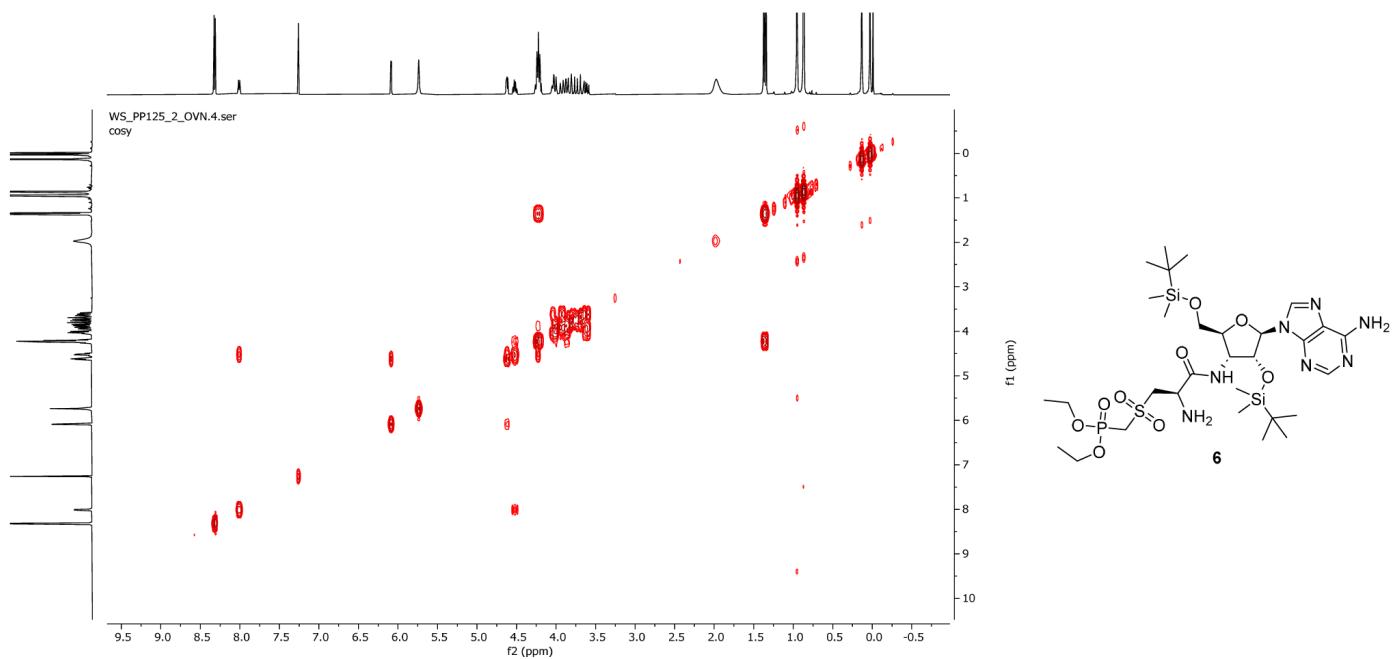
**Fig. S22** <sup>1</sup>H NMR spectrum of compound 6 (400 MHz, CDCl<sub>3</sub>), where ppm = parts per million



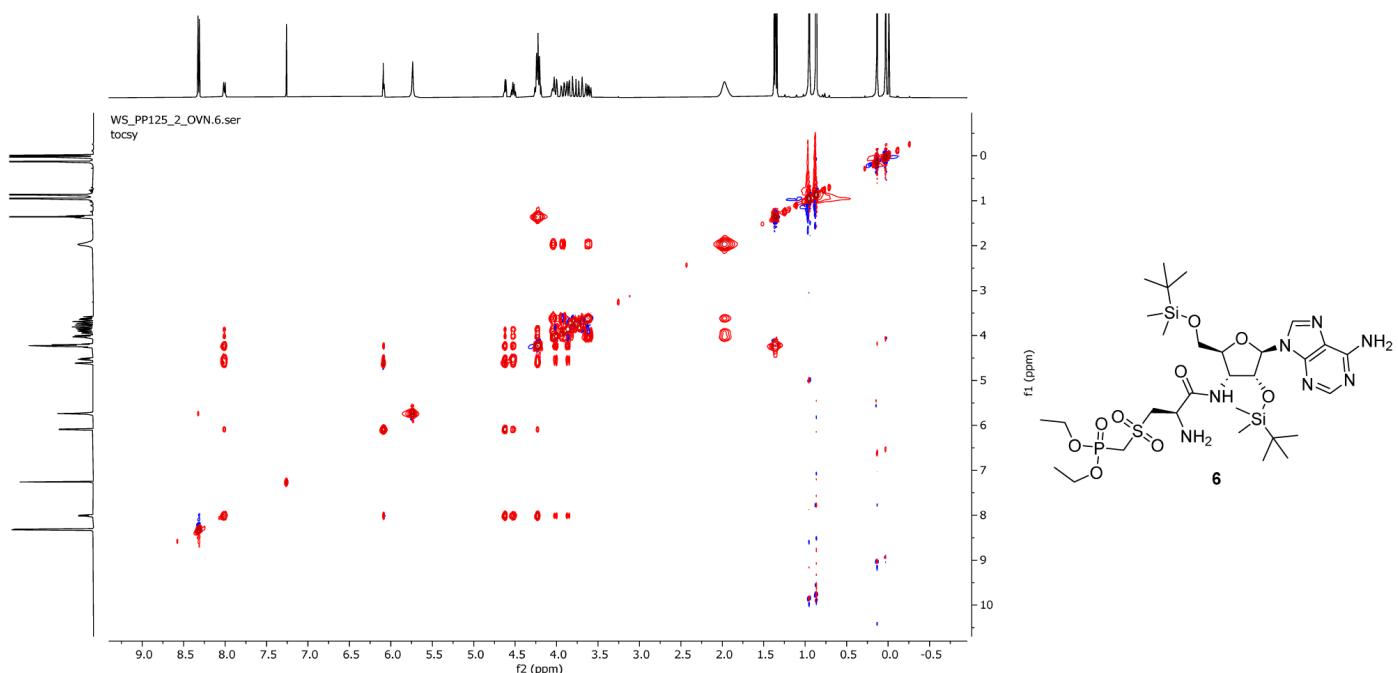
**Fig. S23** <sup>13</sup>C NMR spectrum of compound 6 (100 MHz, CDCl<sub>3</sub>), where ppm = parts per million



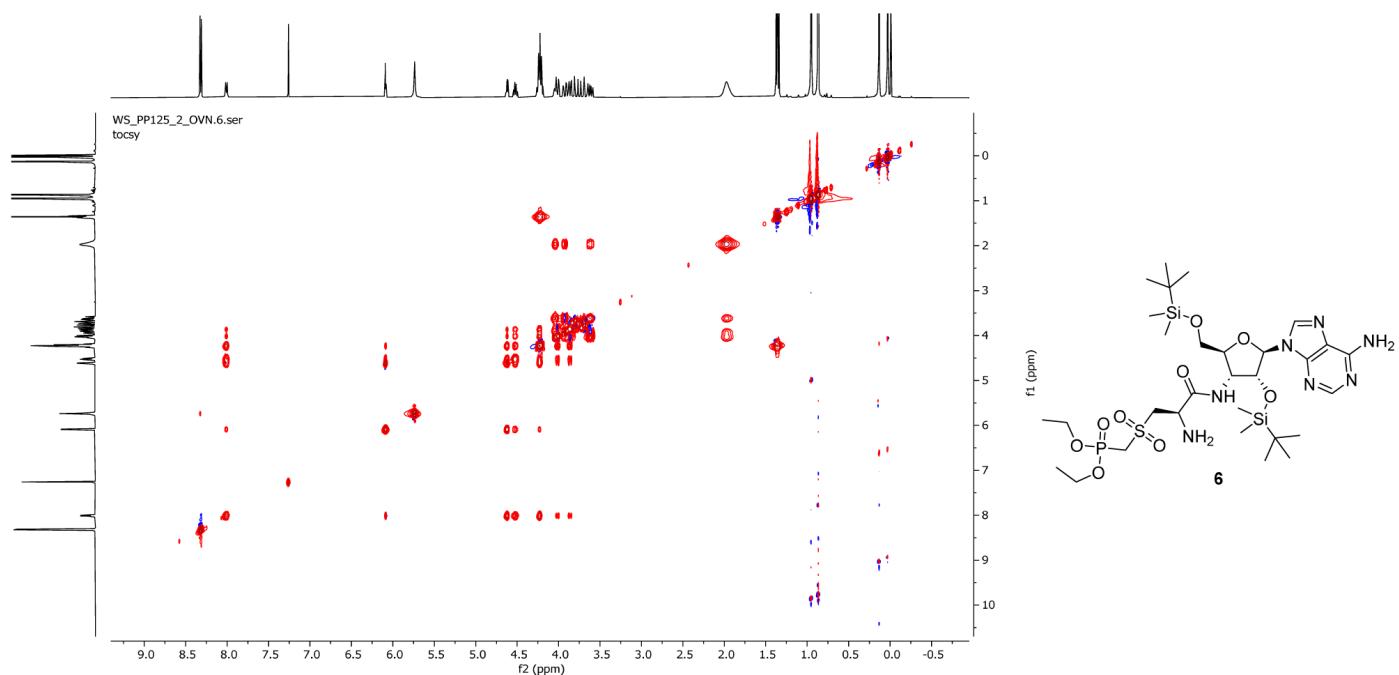
**Fig. S24** DEPT spectra of compound 6 (100 MHz, CDCl<sub>3</sub>), where ppm = parts per million



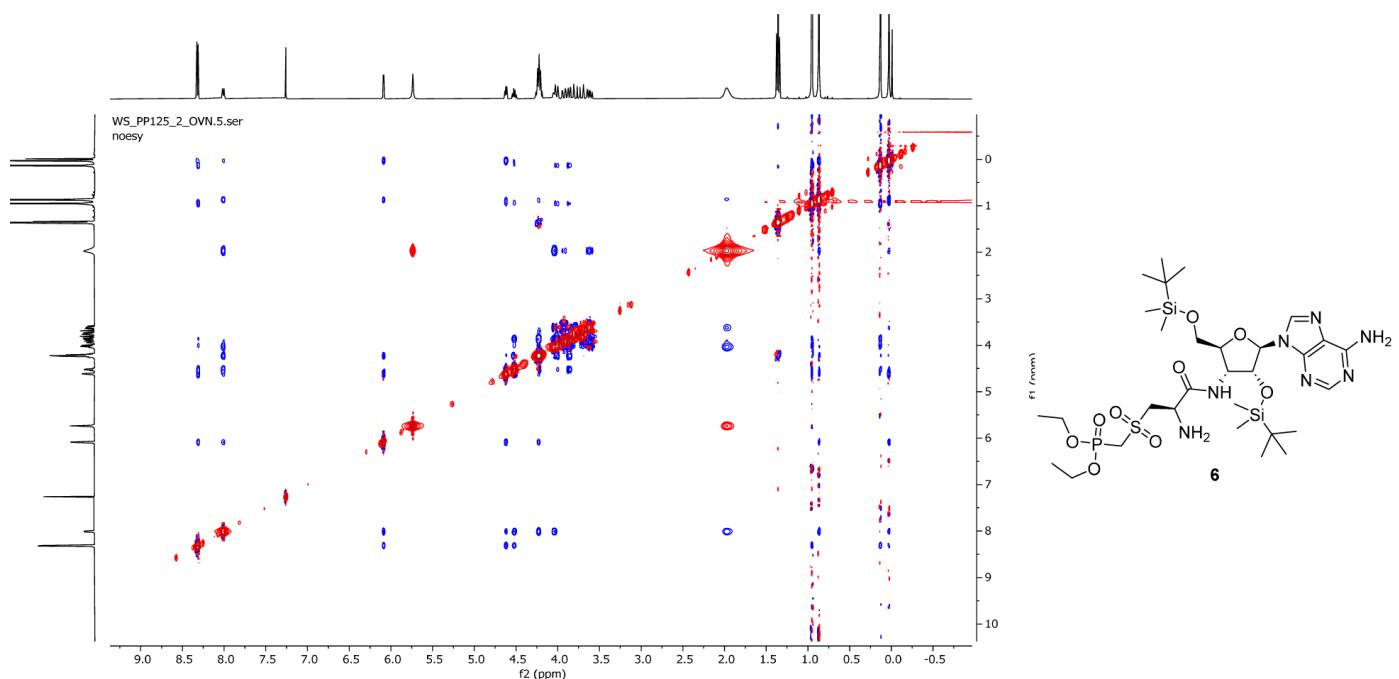
**Fig. S25** COSY spectrum of compound 6 (400 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



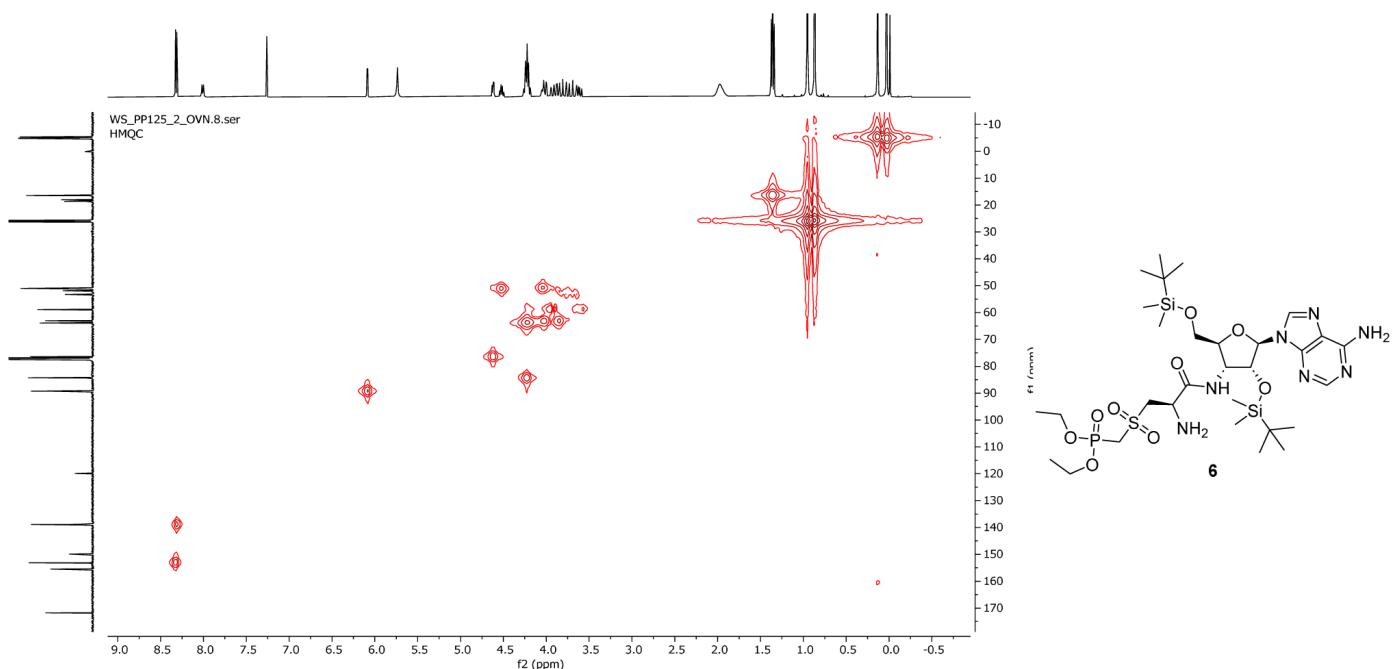
**Fig. S26** TOCSY spectrum of compound 6 (400 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



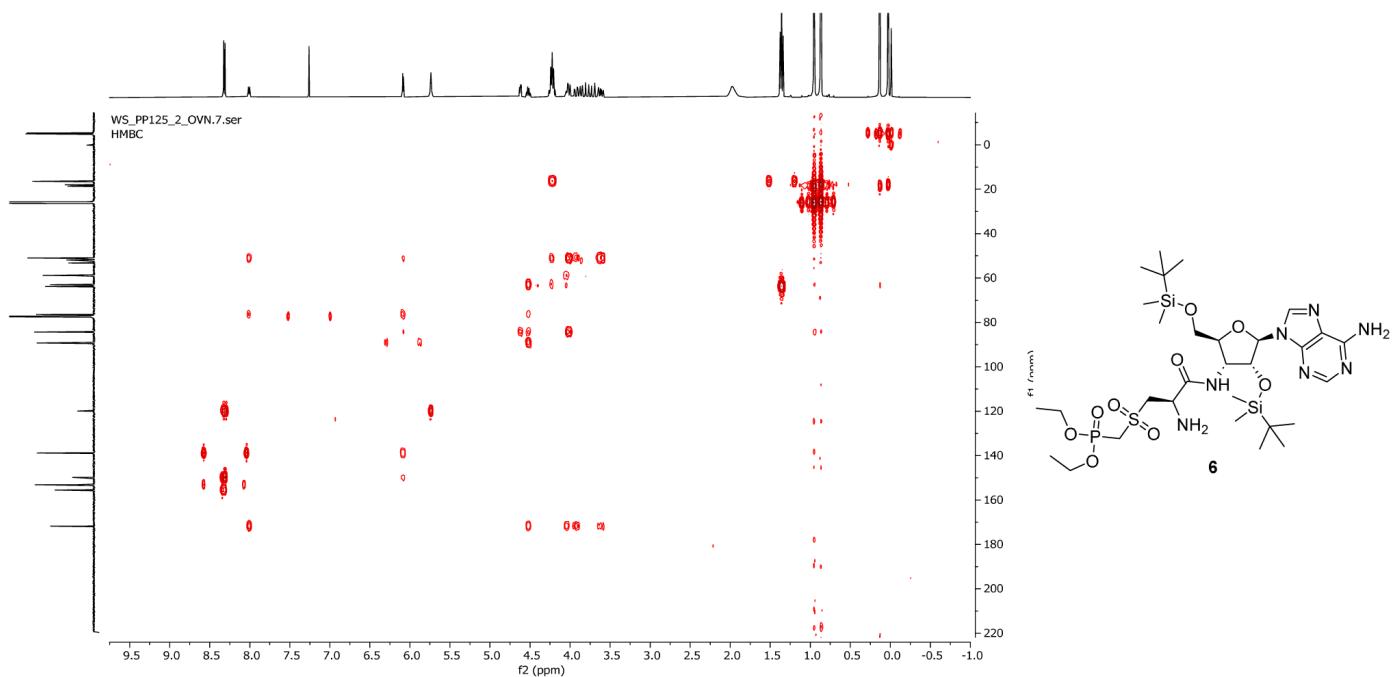
**Fig. S27** NOESY spectrum of compound 6 (400 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



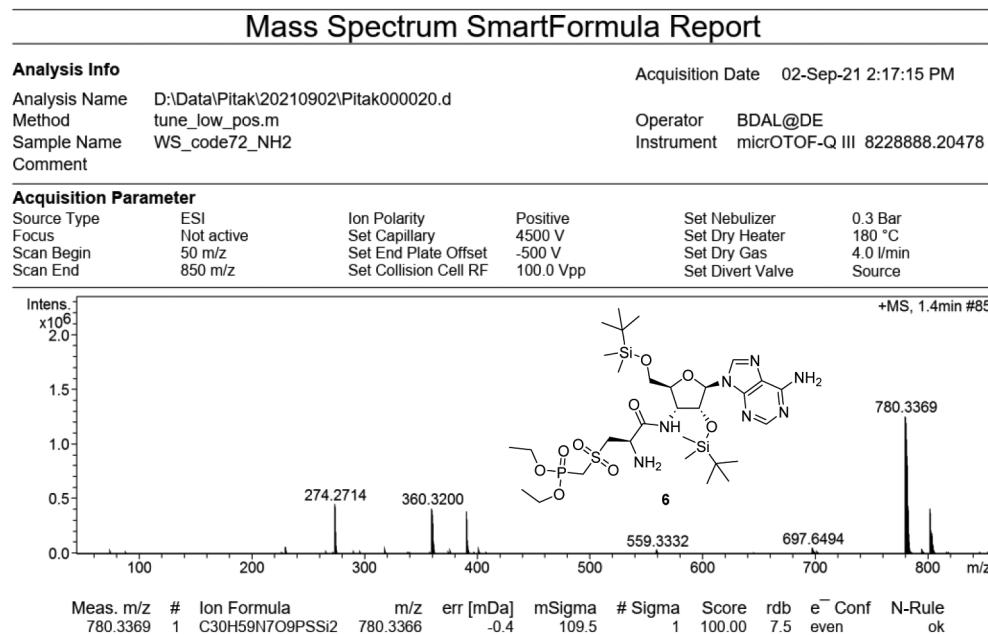
**Fig. S28** HSQC-edited spectrum of compound 6 (400 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



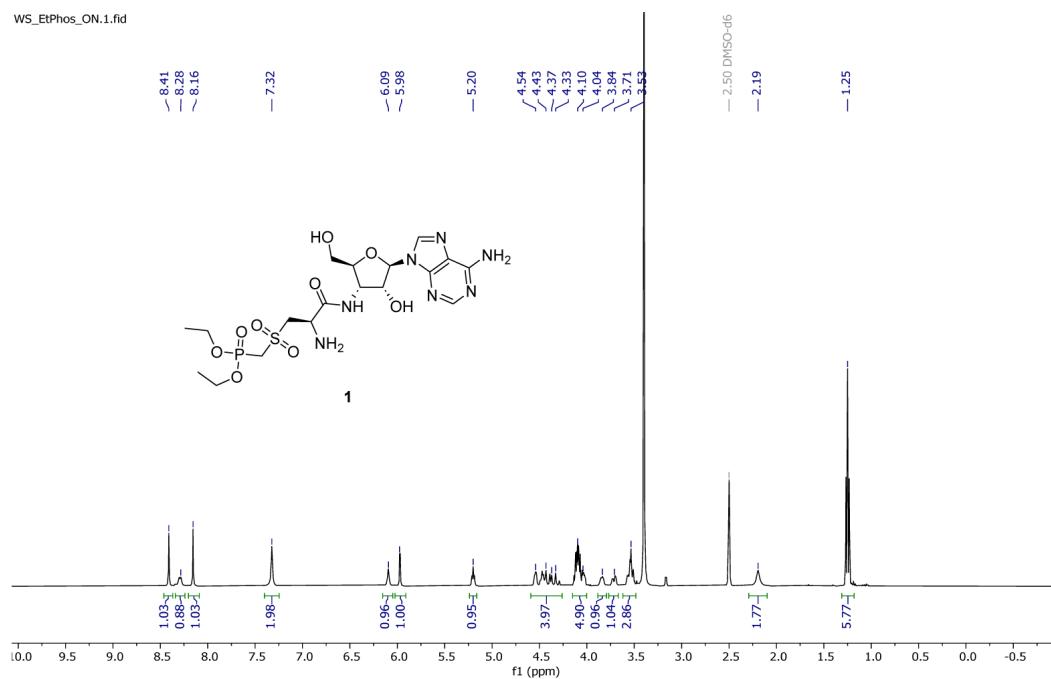
**Fig. S29** HMQC spectrum of compound 6 (400 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



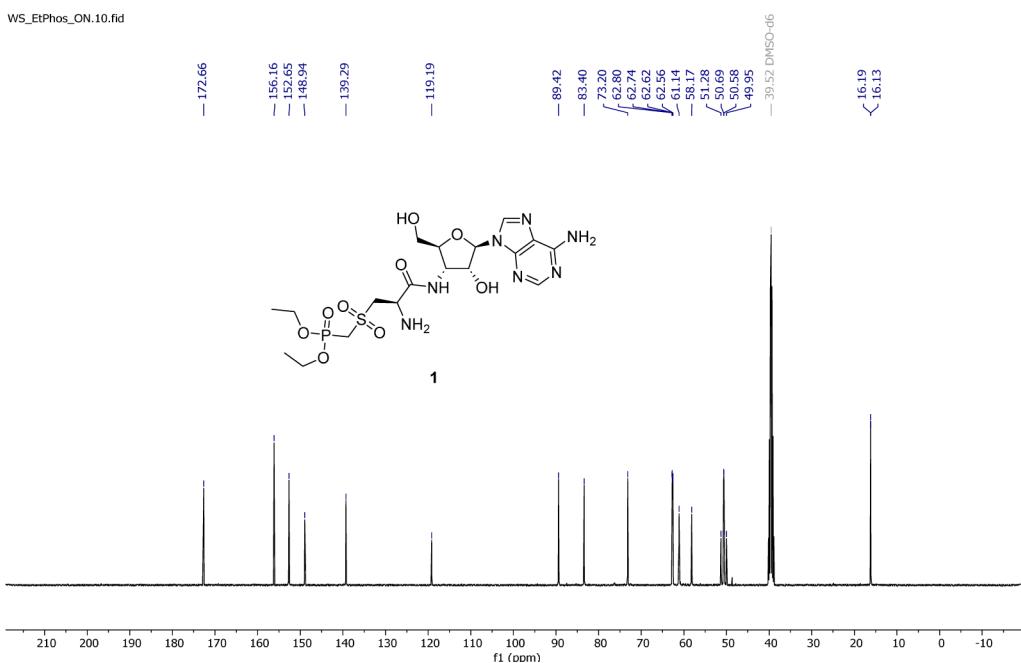
**Fig. S30** HMBC spectrum of compound 6 (400 MHz,  $\text{CDCl}_3$ ), where ppm = parts per million



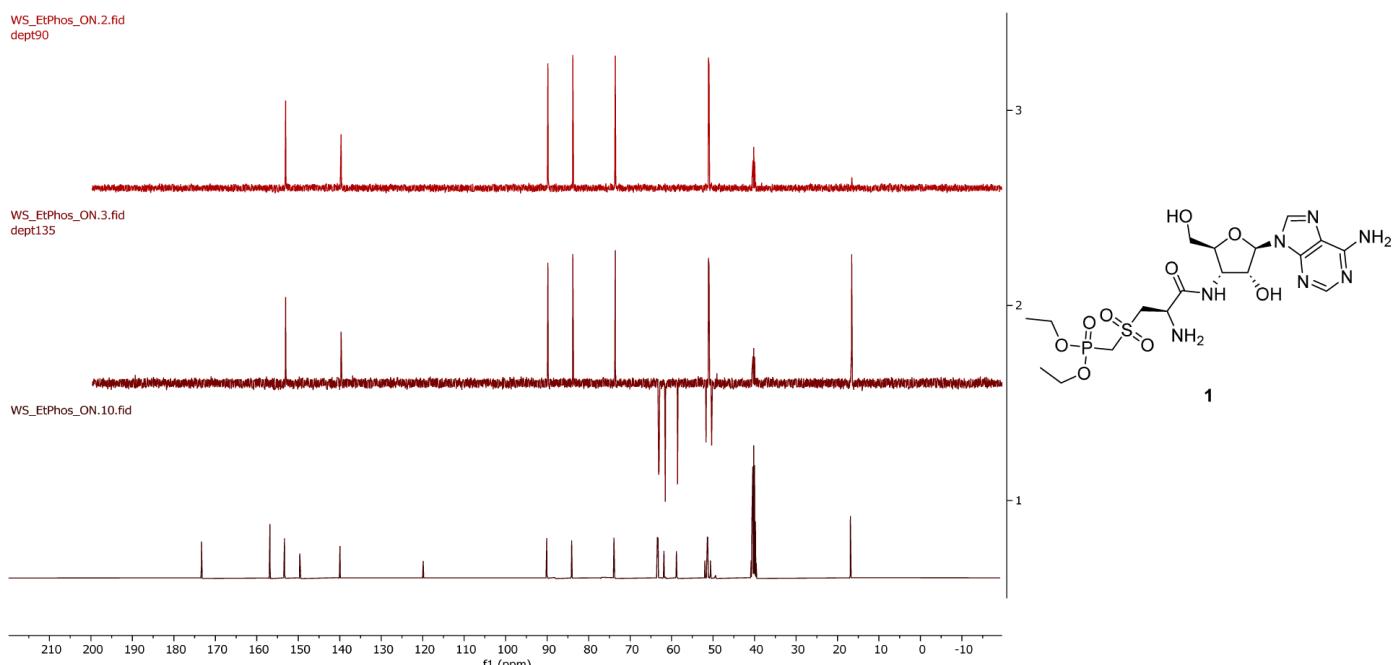
**Fig. S31** High-resolution mass spectrum (HRMS) of compound 6



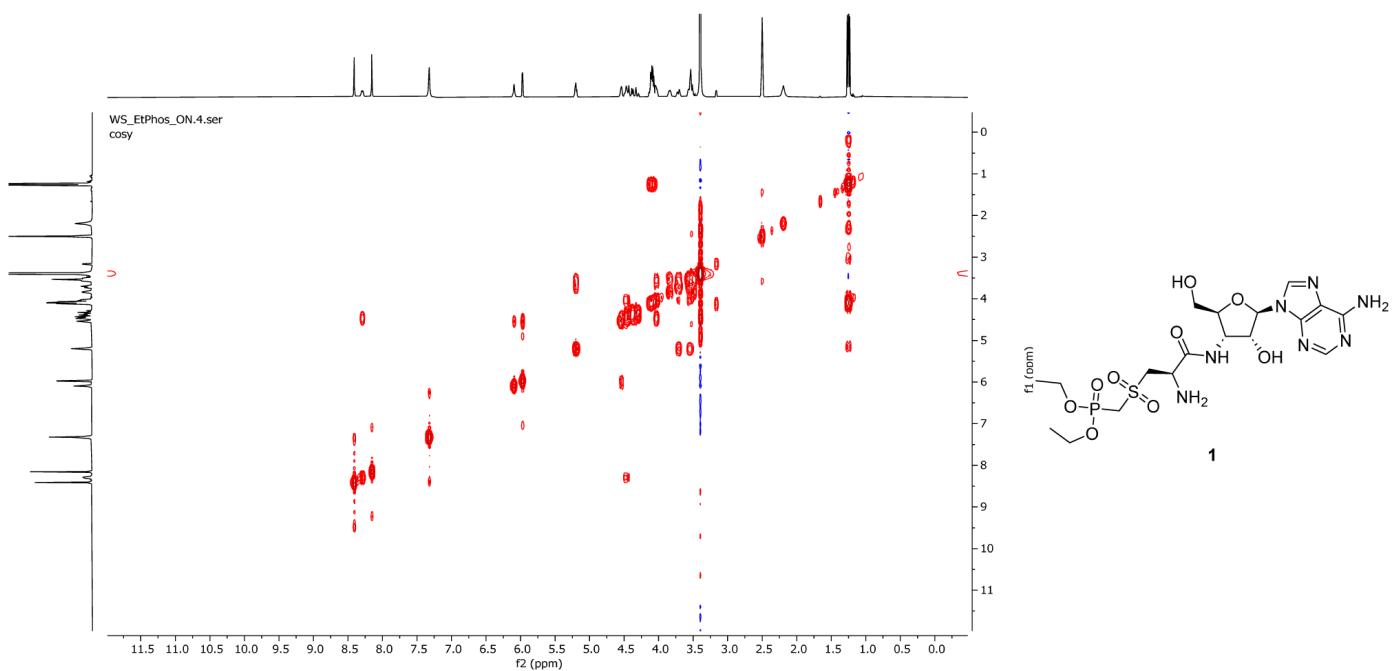
**Fig. S32** <sup>1</sup>H NMR spectrum of compound 1 (400 MHz, DMSO-*d*<sub>6</sub>), where ppm = parts per million



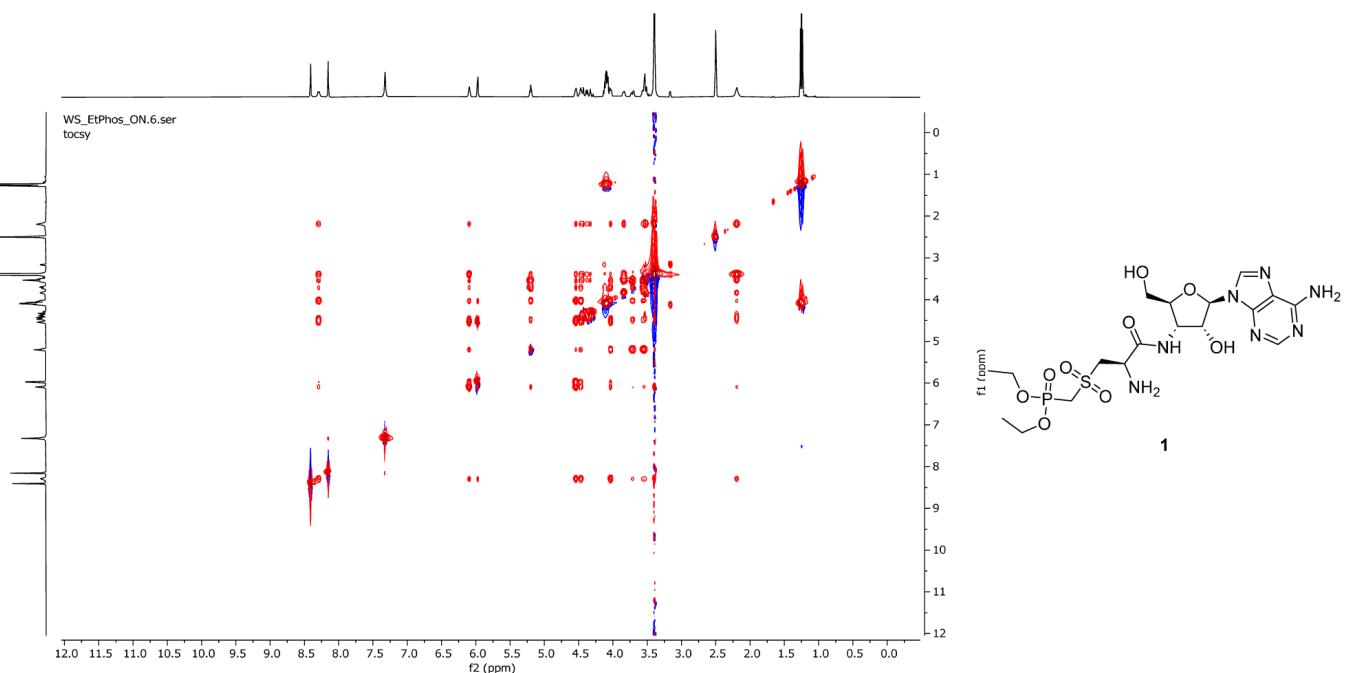
**Fig. S33**  $^{13}\text{C}$  NMR spectrum of compound 1 (100 MHz,  $\text{DMSO}-d_6$ ), where ppm = parts per million



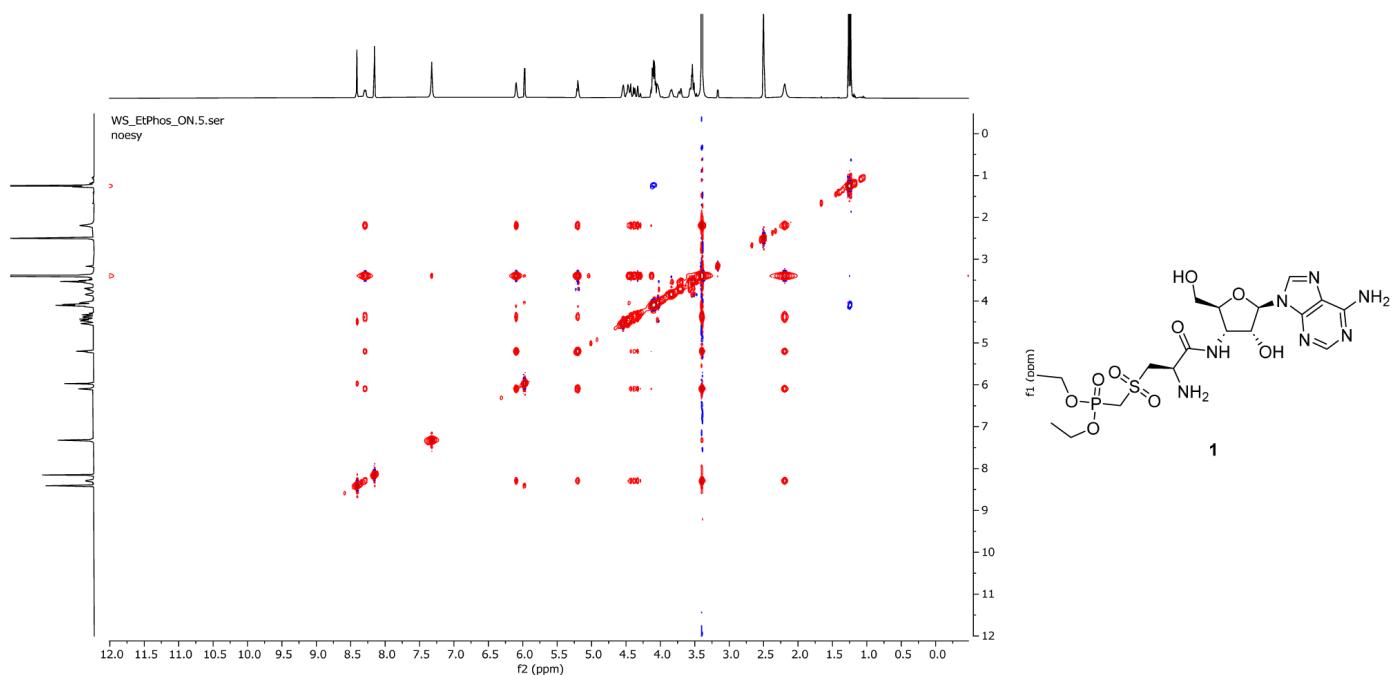
**Fig. S34** DEPT spectra of compound 1 (100 MHz,  $\text{DMSO}-d_6$ ), where ppm = parts per million



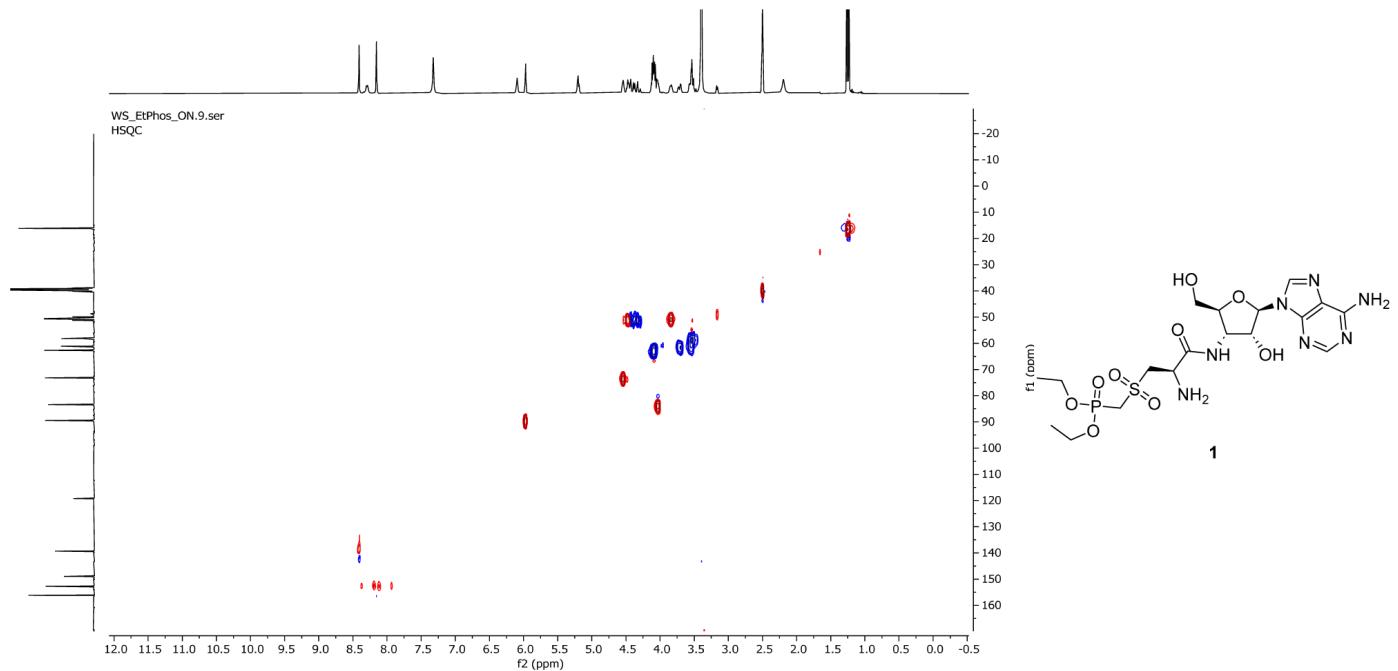
**Fig. S35** COSY spectrum of compound 1 (400 MHz,  $\text{DMSO}-d_6$ ), where ppm = parts per million



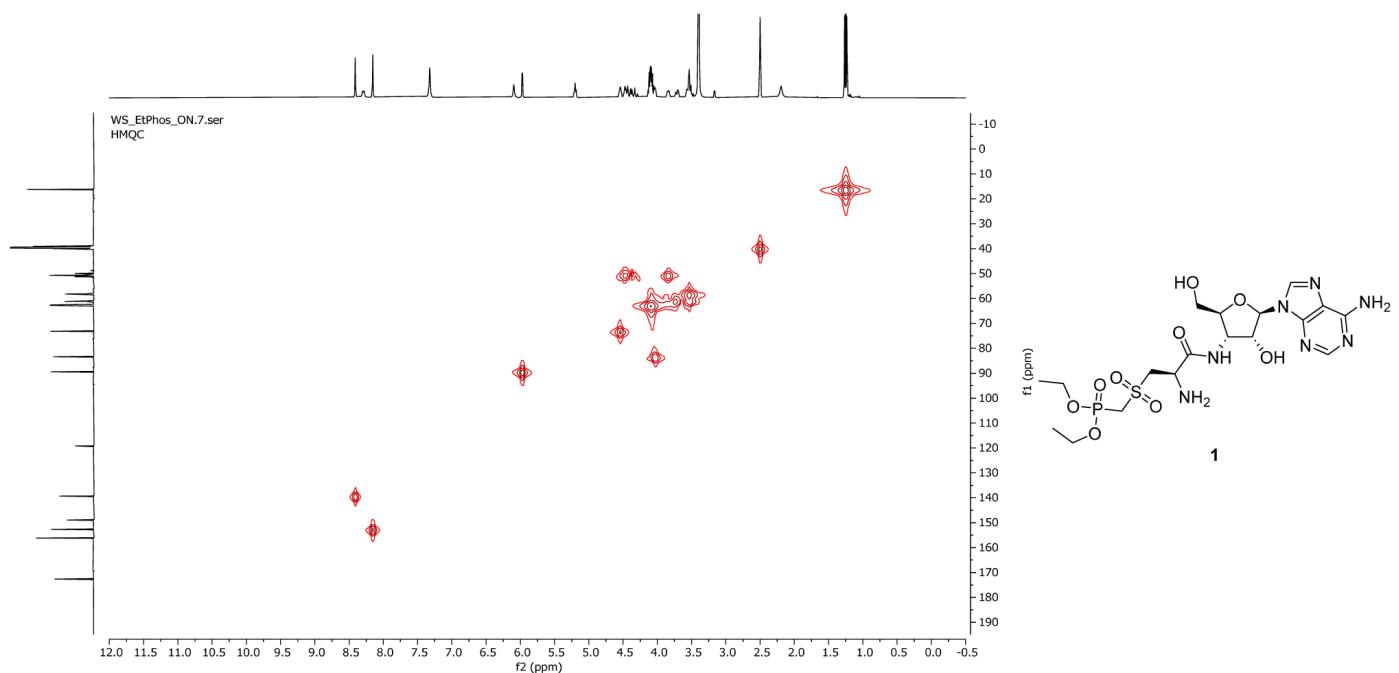
**Fig. S36** TOCSY spectrum of compound 1 (400 MHz,  $\text{DMSO}-d_6$ ), where ppm = parts per million



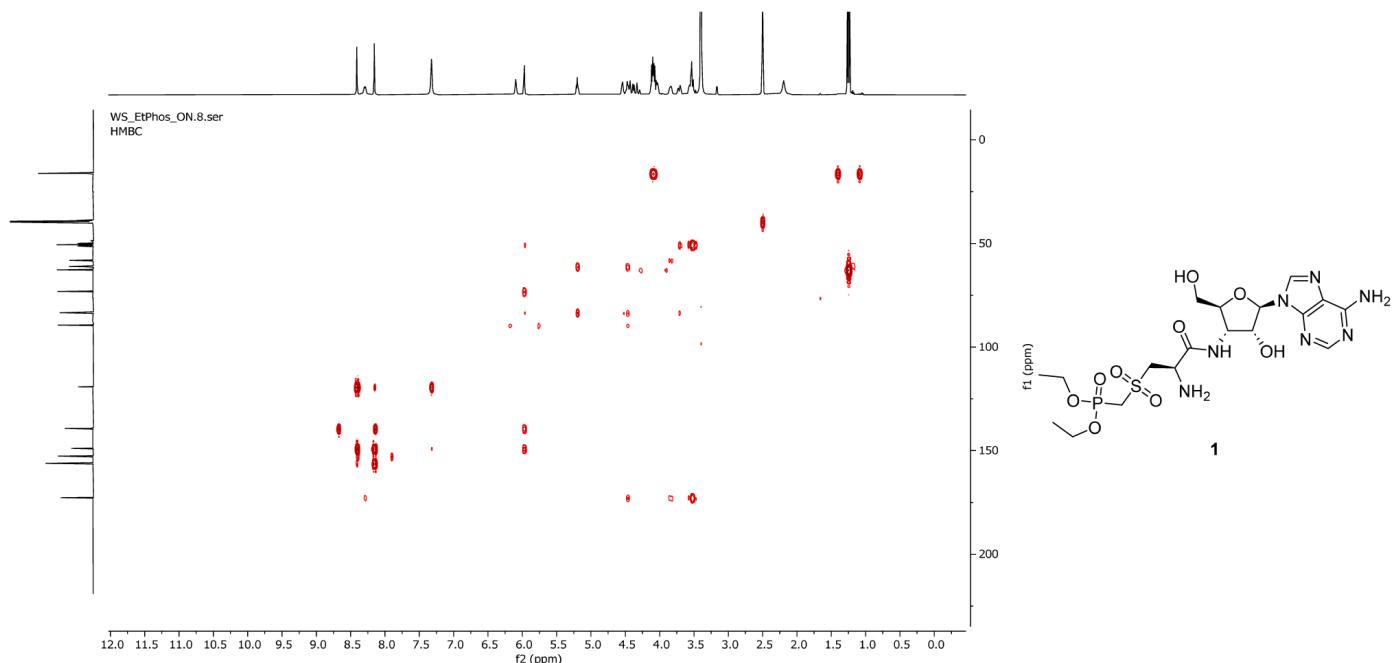
**Fig. S37** NOESY spectrum of compound 1 (400 MHz,  $\text{DMSO-}d_6$ ), where ppm = parts per million



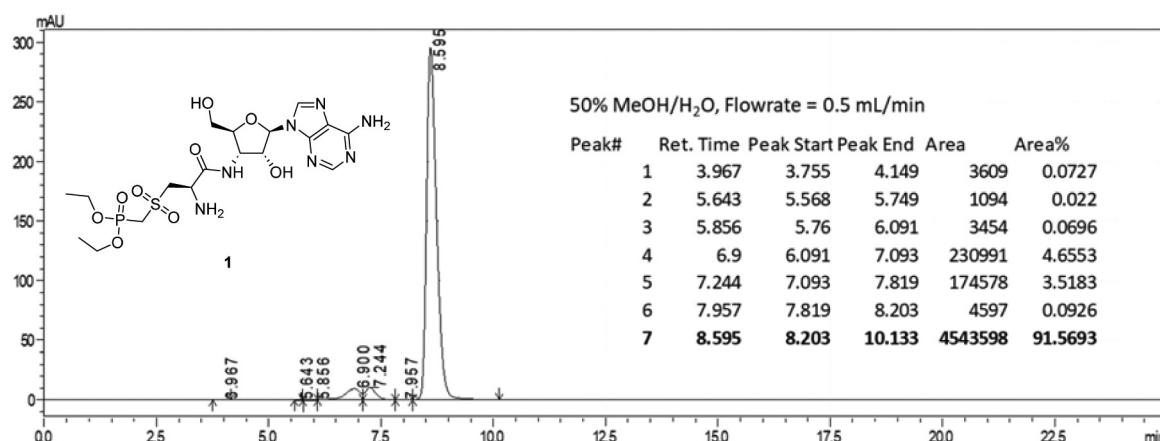
**Fig. S38** HSQC-edited spectrum of compound 1 (400 MHz,  $\text{DMSO-}d_6$ ), where ppm = parts per million



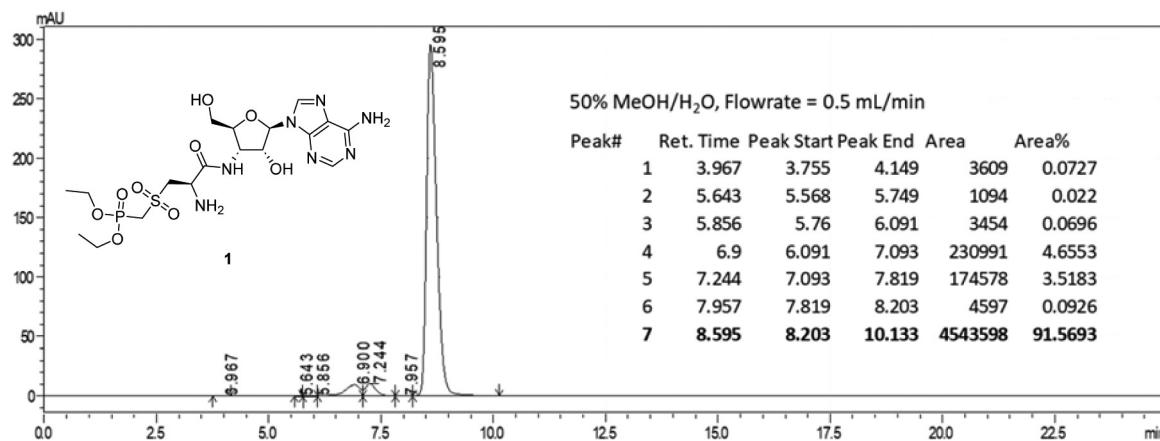
**Fig. S39** HMQC spectrum of compound 1 (400 MHz,  $\text{DMSO}-d_6$ ), where ppm = parts per million



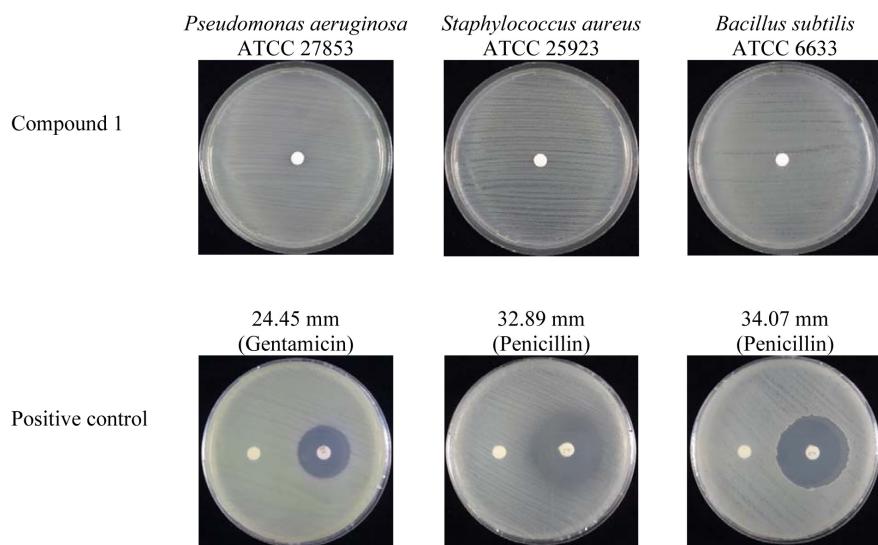
**Fig. S40** HMBC spectrum of compound 1 (400 MHz,  $\text{DMSO}-d_6$ ), where ppm = parts per million



**Fig. S41** High-resolution mass spectrum (HRMS) of compound 1



**Fig. S42** HPLC trace chromatogram of compound 1



**Fig. S43** Disc diffusion antibacterial results