

**Designing of potent Tyrosinase Inhibiting *N*-Arylated-4-yl-benzamides bearing 2-aminothiazole-triazole bi-heterocycles: Mechanistic Insight through Enzyme Inhibition, Kinetics and Computational Studies.**

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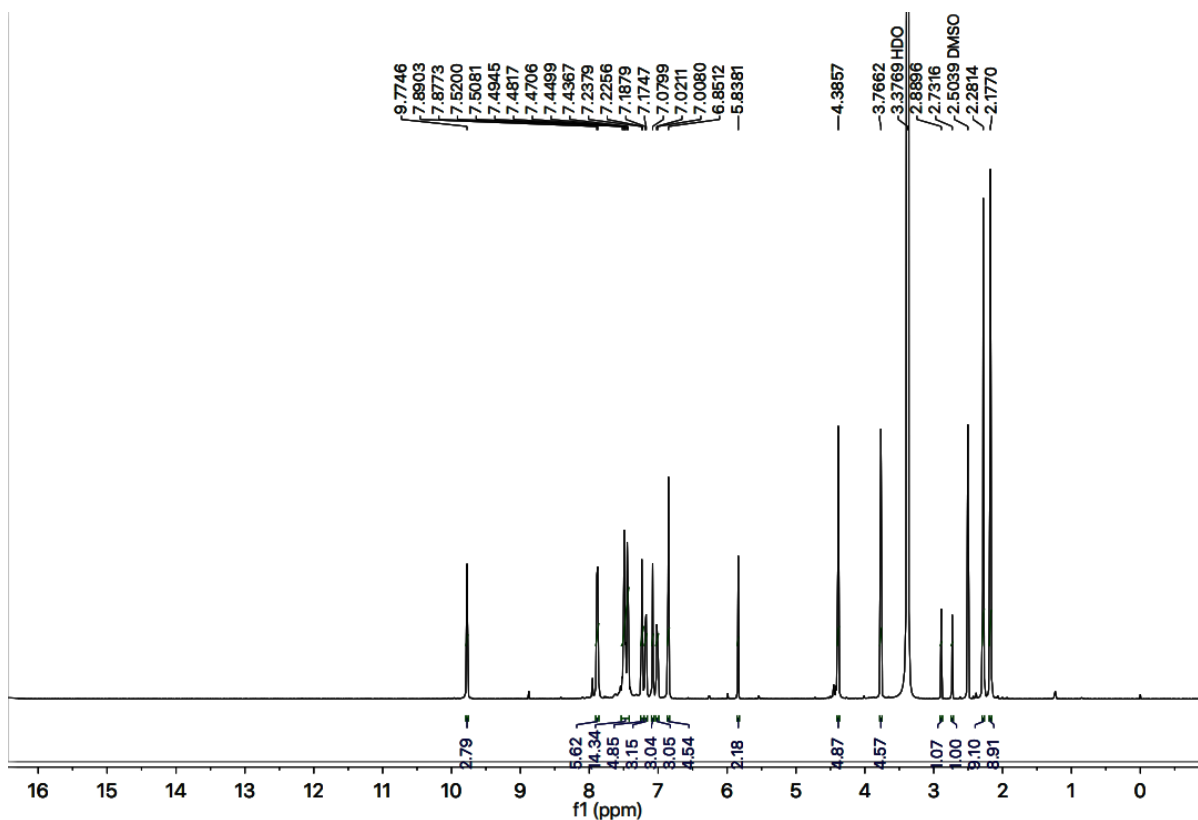


FIGURE S1 <sup>1</sup>H-NMR spectrum of 9a

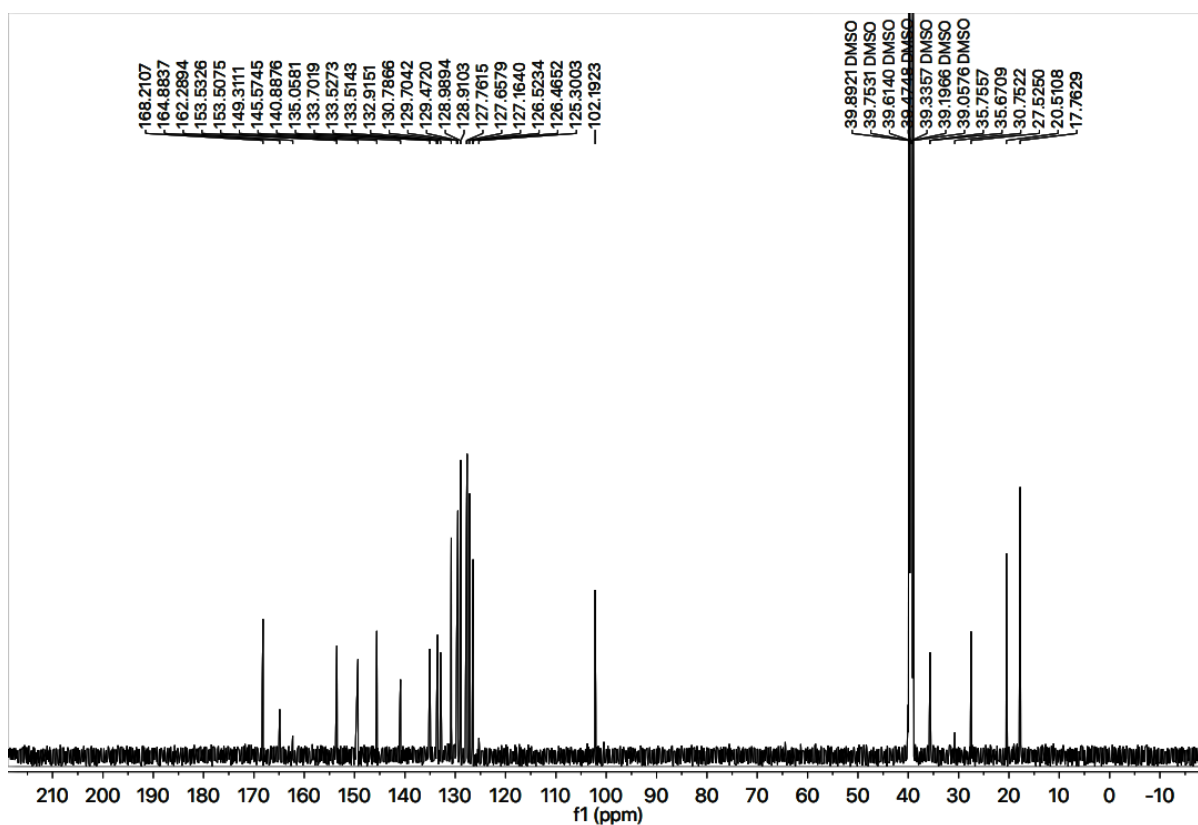


FIGURE S2 <sup>13</sup>C-NMR spectrum of 9a

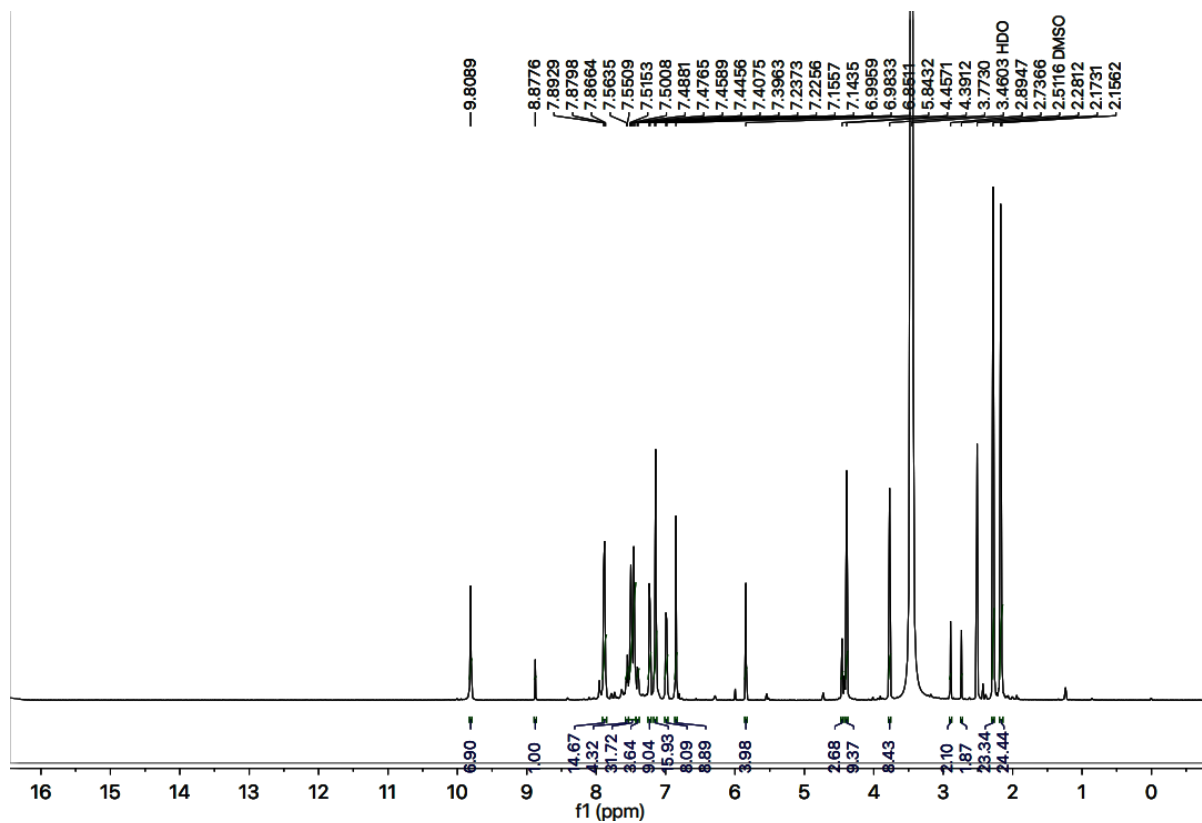


FIGURE S3  $^1\text{H-NMR}$  spectrum of **9b**

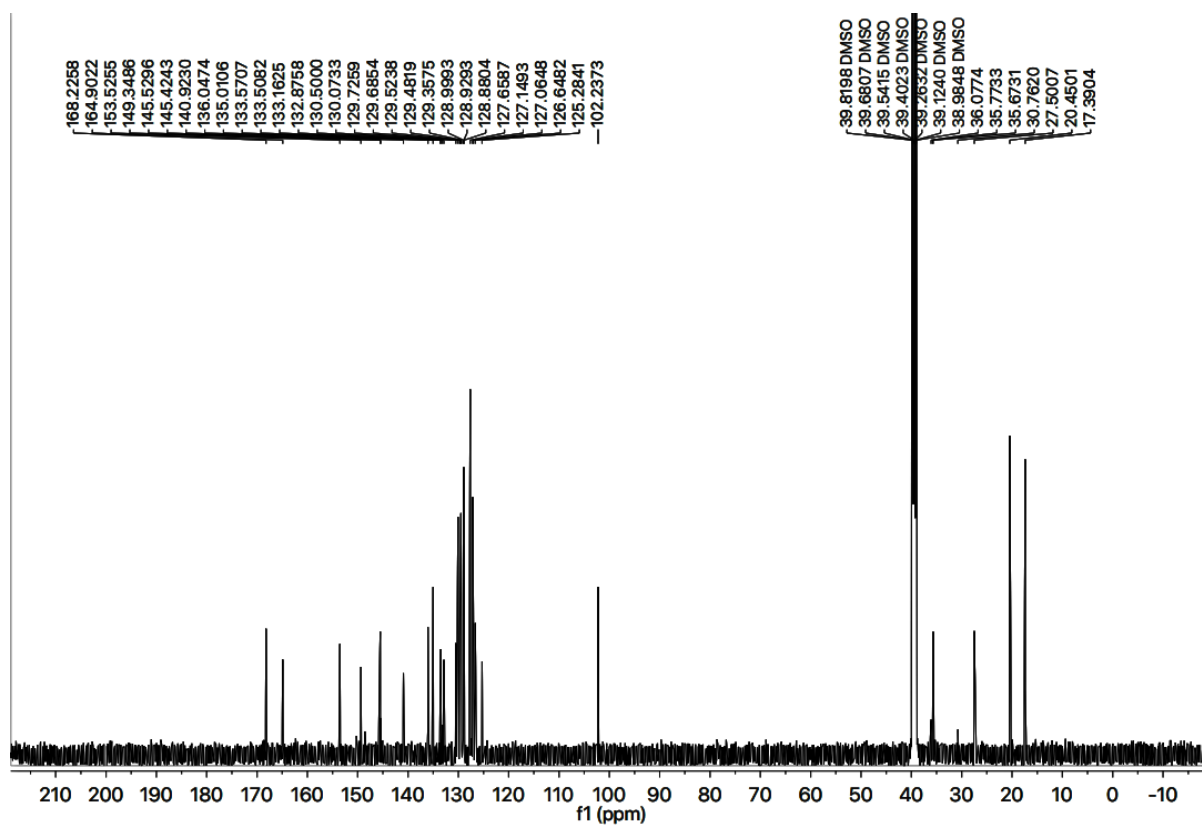


FIGURE S4  $^{13}\text{C-NMR}$  spectrum of **9b**

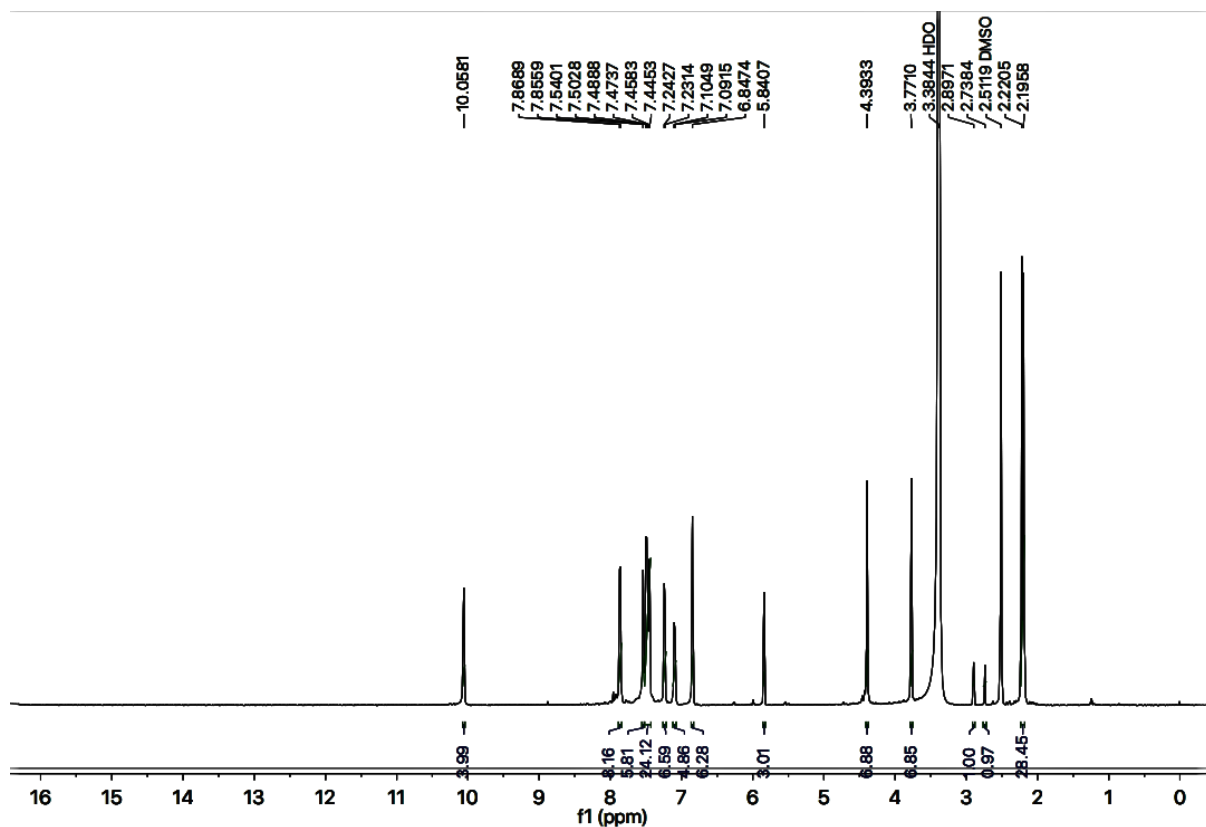


FIGURE S5 <sup>1</sup>H-NMR spectrum of 9d

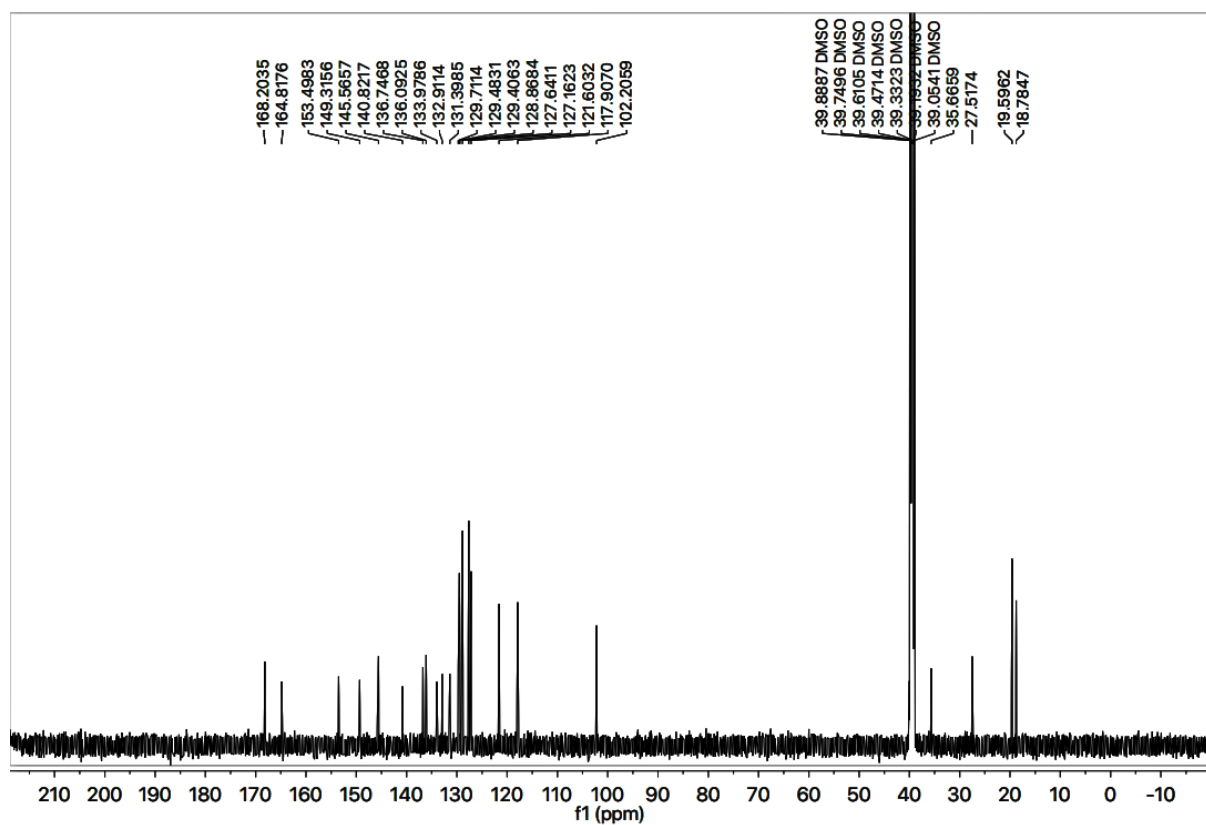


FIGURE S6 <sup>13</sup>C-NMR spectrum of 9d

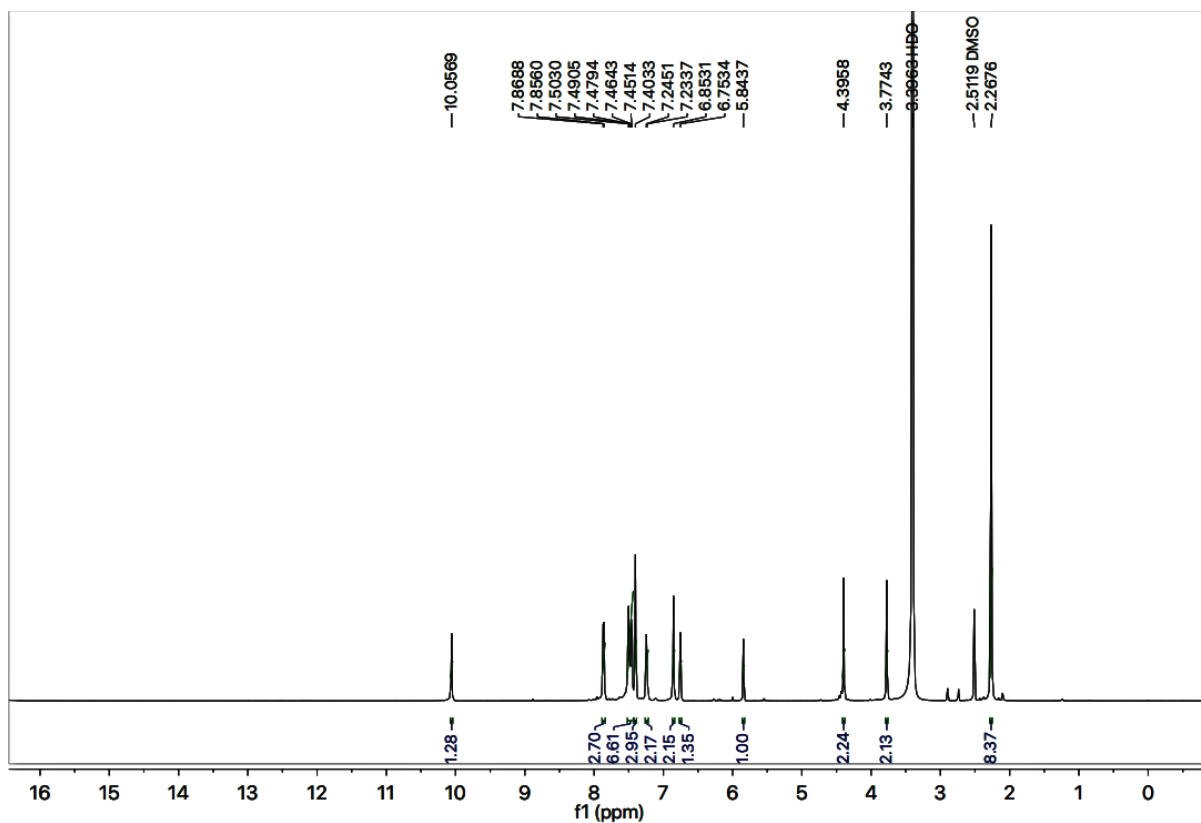


FIGURE S7 <sup>1</sup>H-NMR spectrum of **9e**

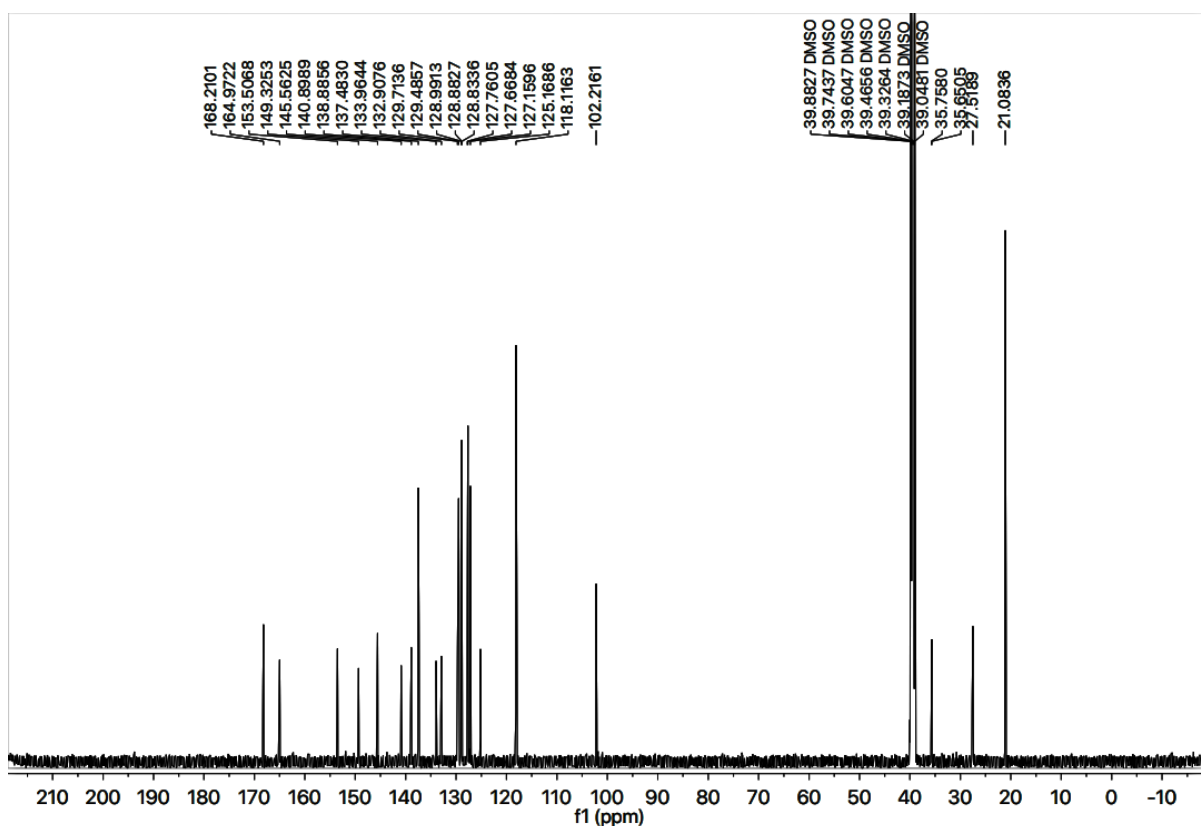


FIGURE S8 <sup>13</sup>C-NMR spectrum of **9e**

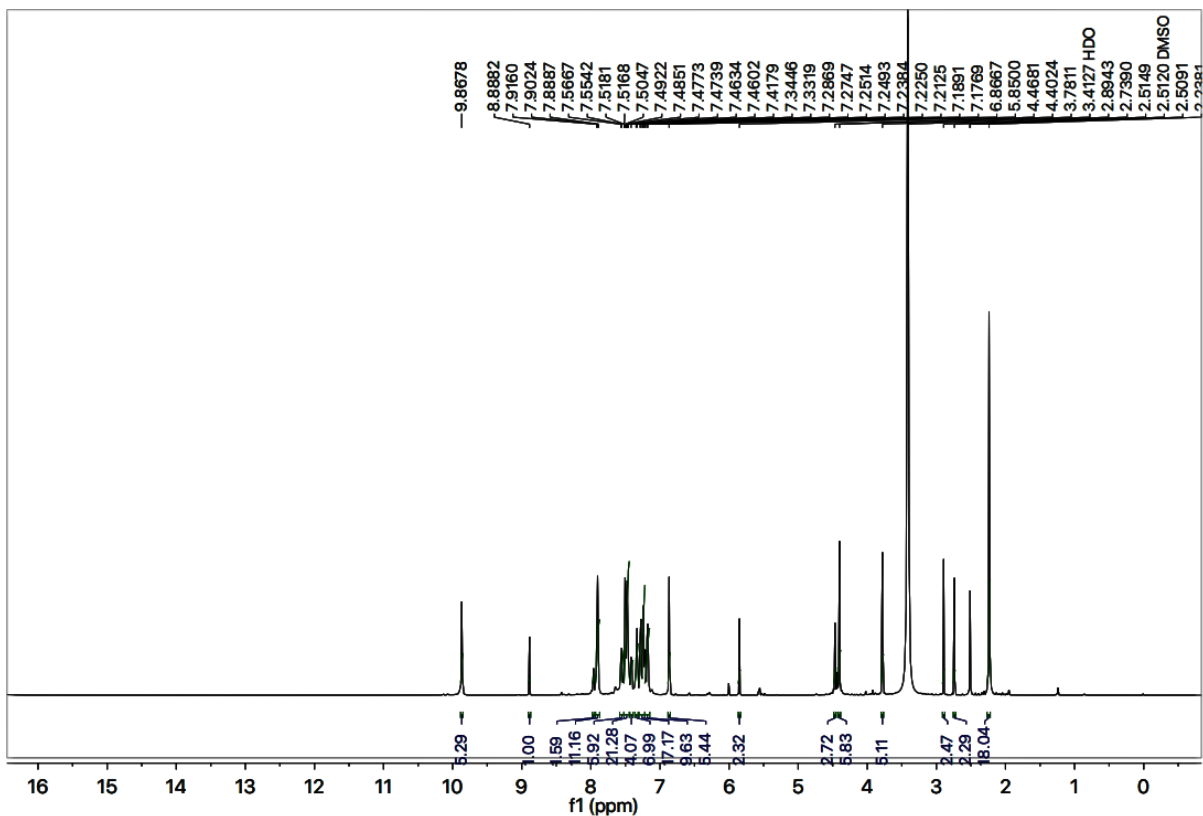


FIGURE S9 <sup>1</sup>H-NMR spectrum of **9f**

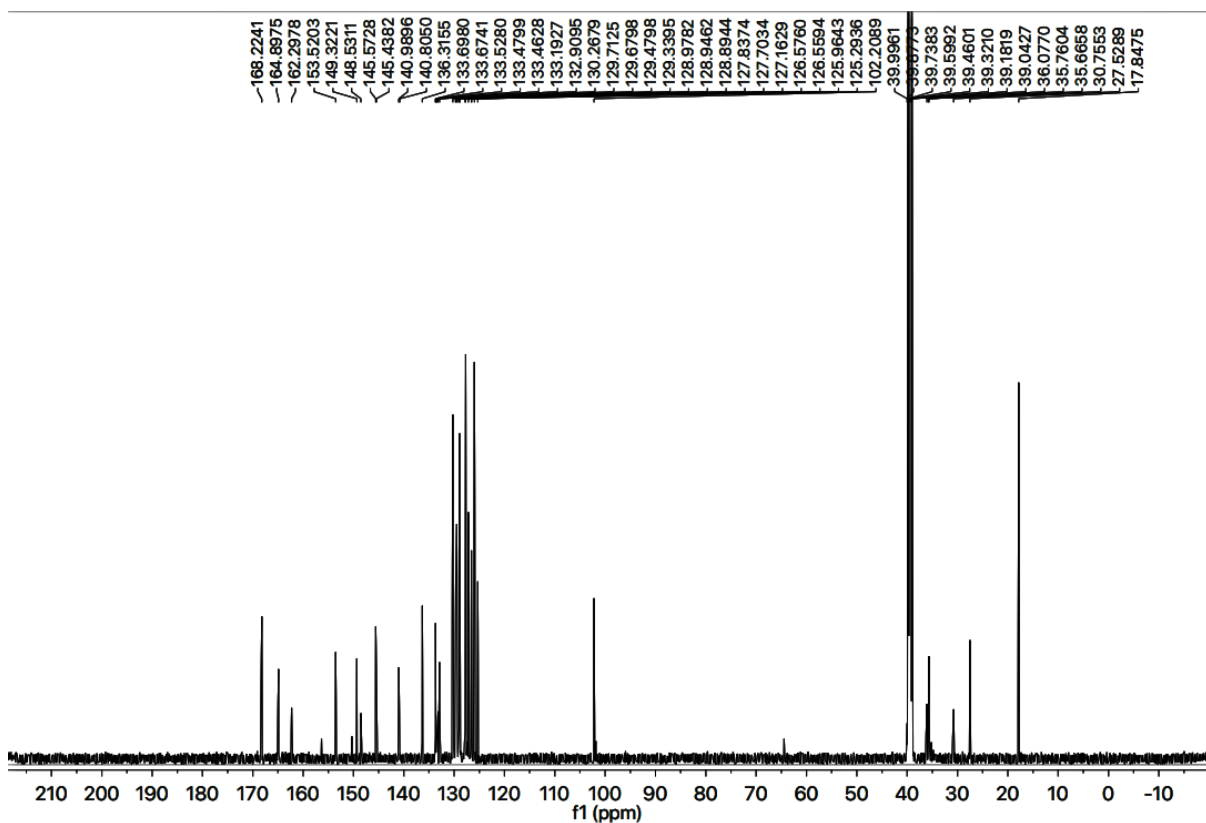


FIGURE S10 <sup>13</sup>C-NMR spectrum of **9f**

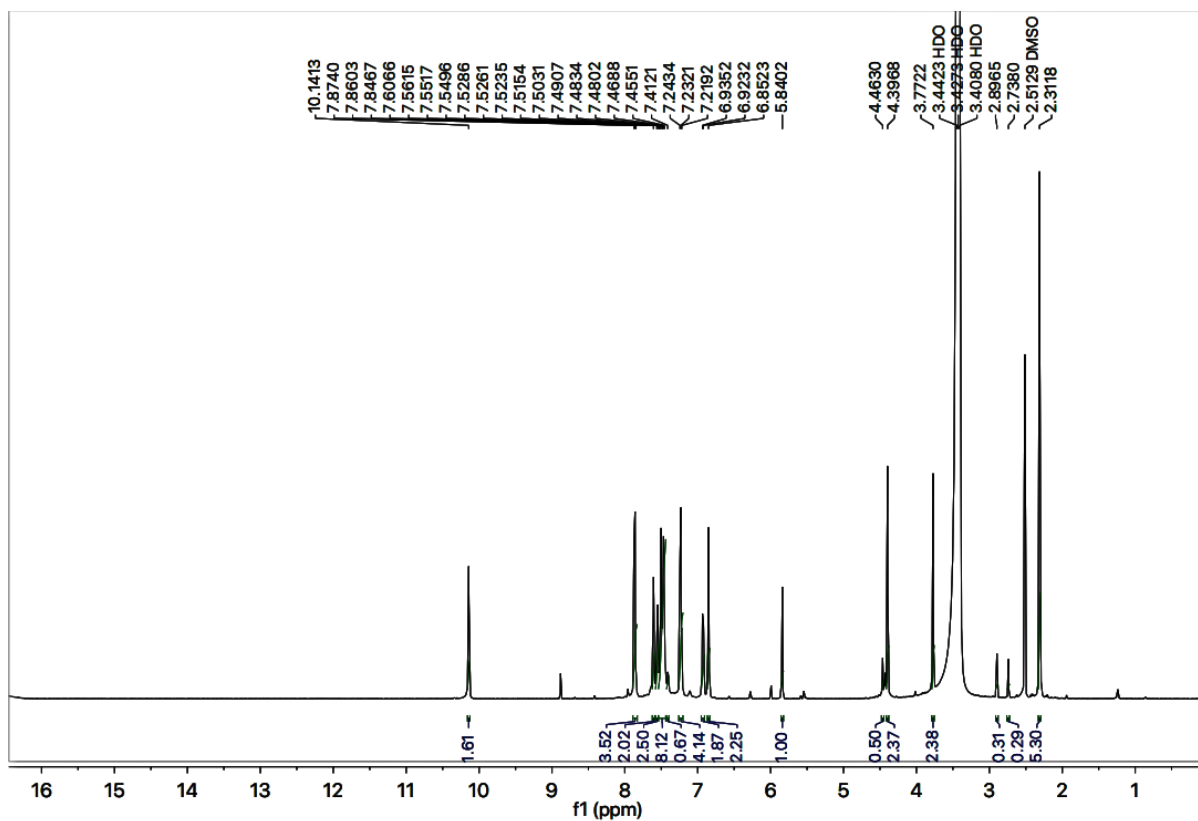


FIGURE S11  $^1\text{H}$ -NMR spectrum of **9g**

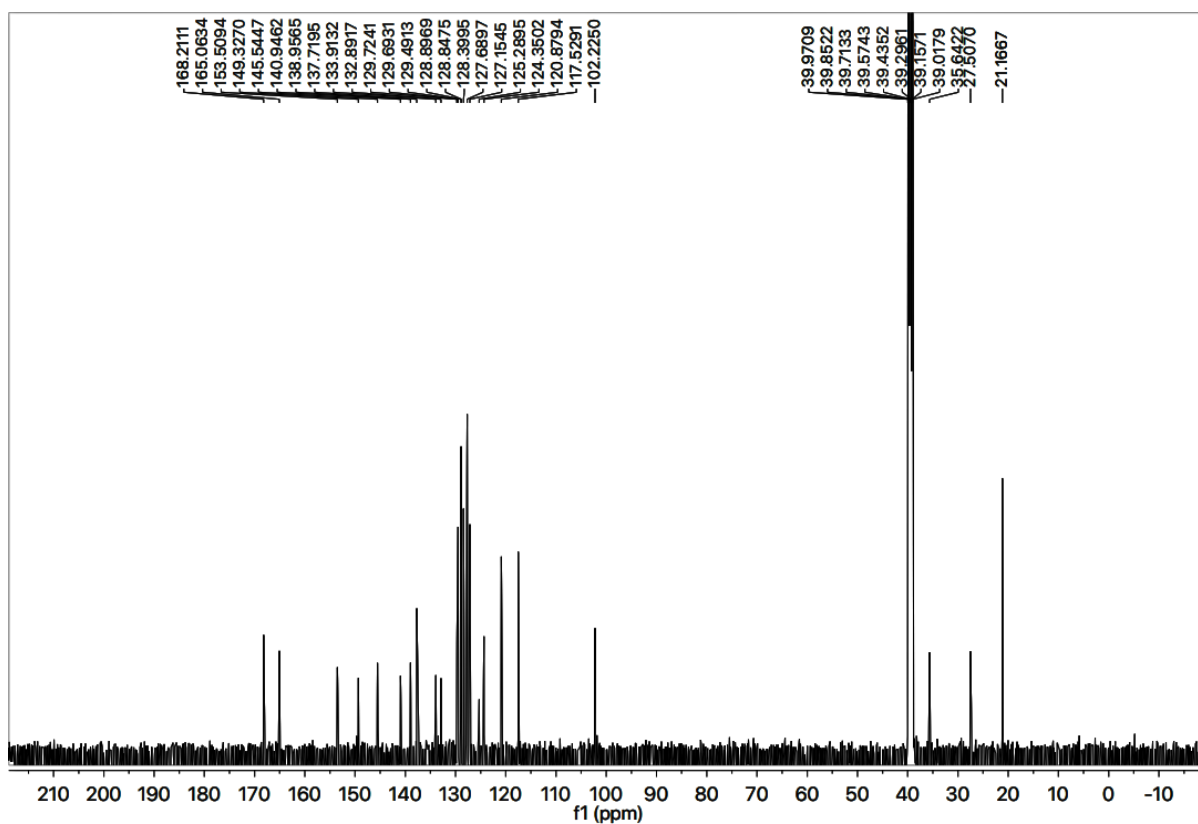


FIGURE S12  $^{13}\text{C}$ -NMR spectrum of **9g**

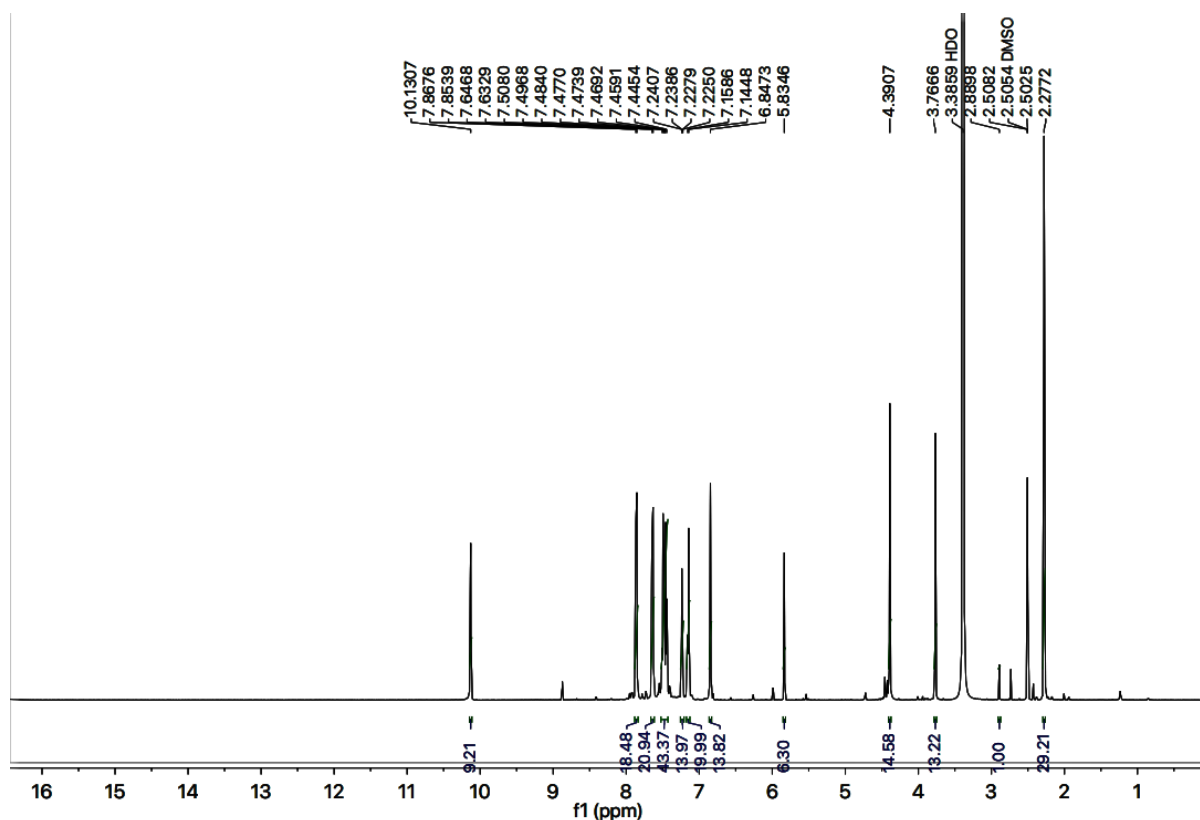


FIGURE S13 <sup>1</sup>H-NMR spectrum of 9h

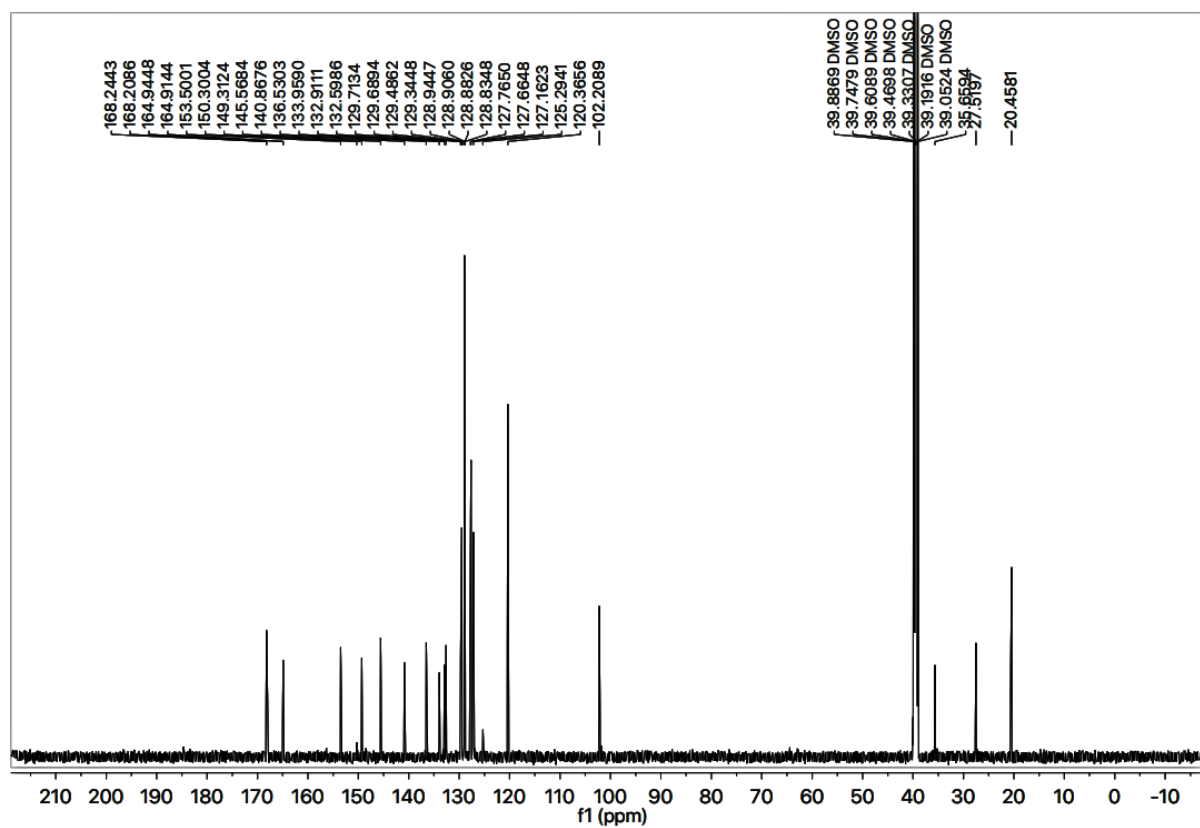


FIGURE S14 <sup>13</sup>C-NMR spectrum of 9h



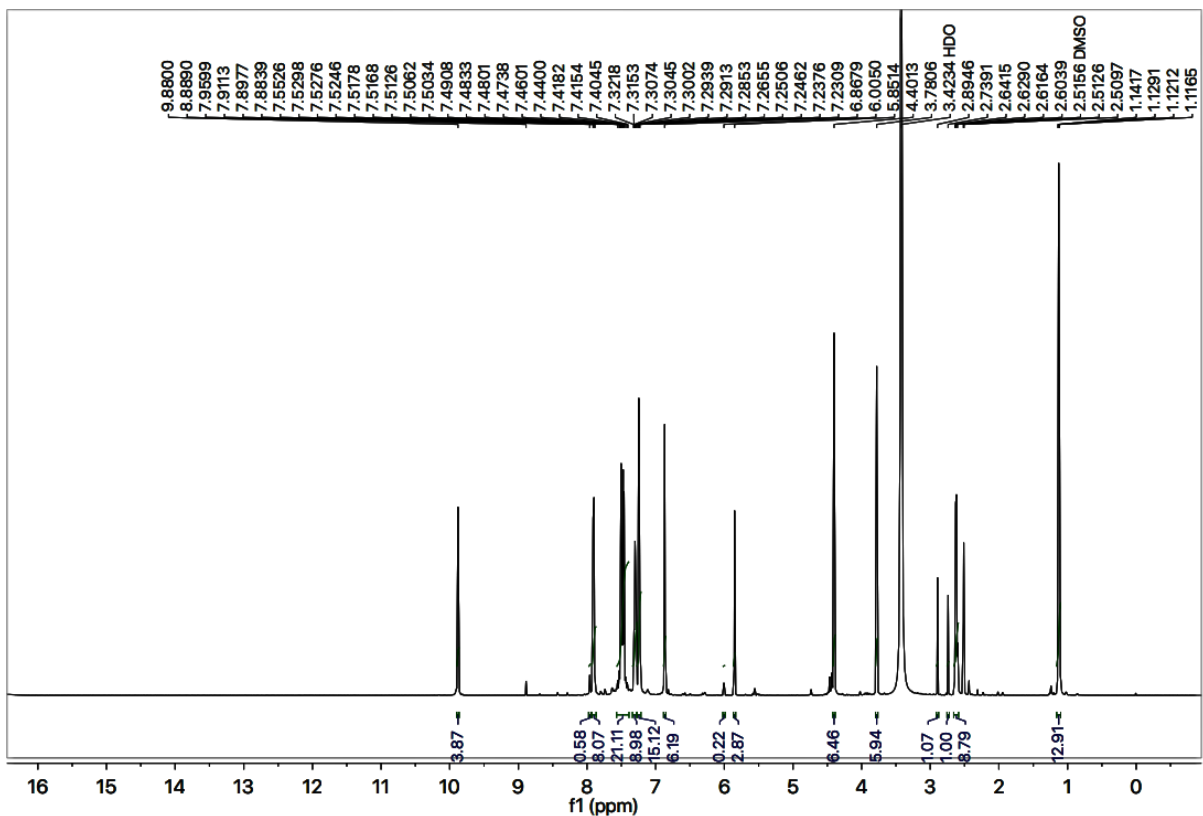


FIGURE S15 <sup>1</sup>H-NMR spectrum of **9i**

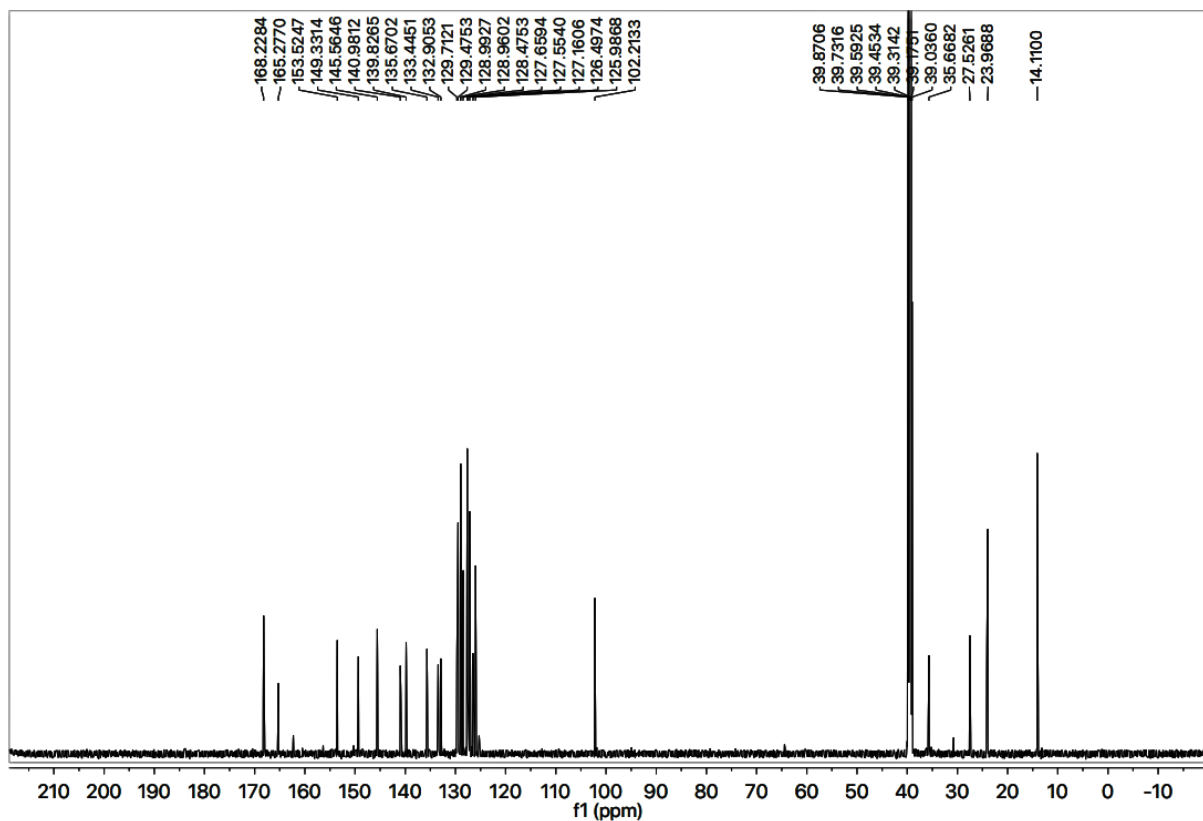


FIGURE S16 <sup>13</sup>C-NMR spectrum of **9i**

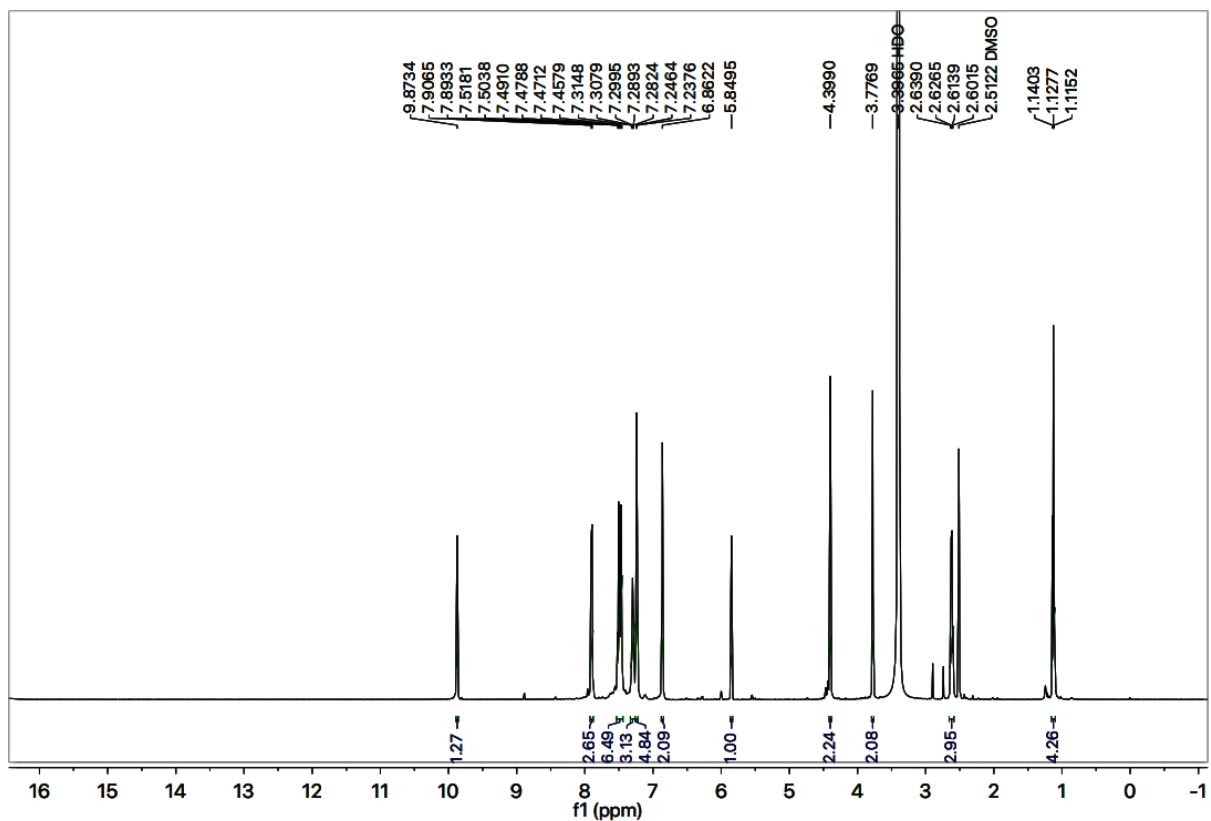


FIGURE S17 <sup>1</sup>H-NMR spectrum of **9j**

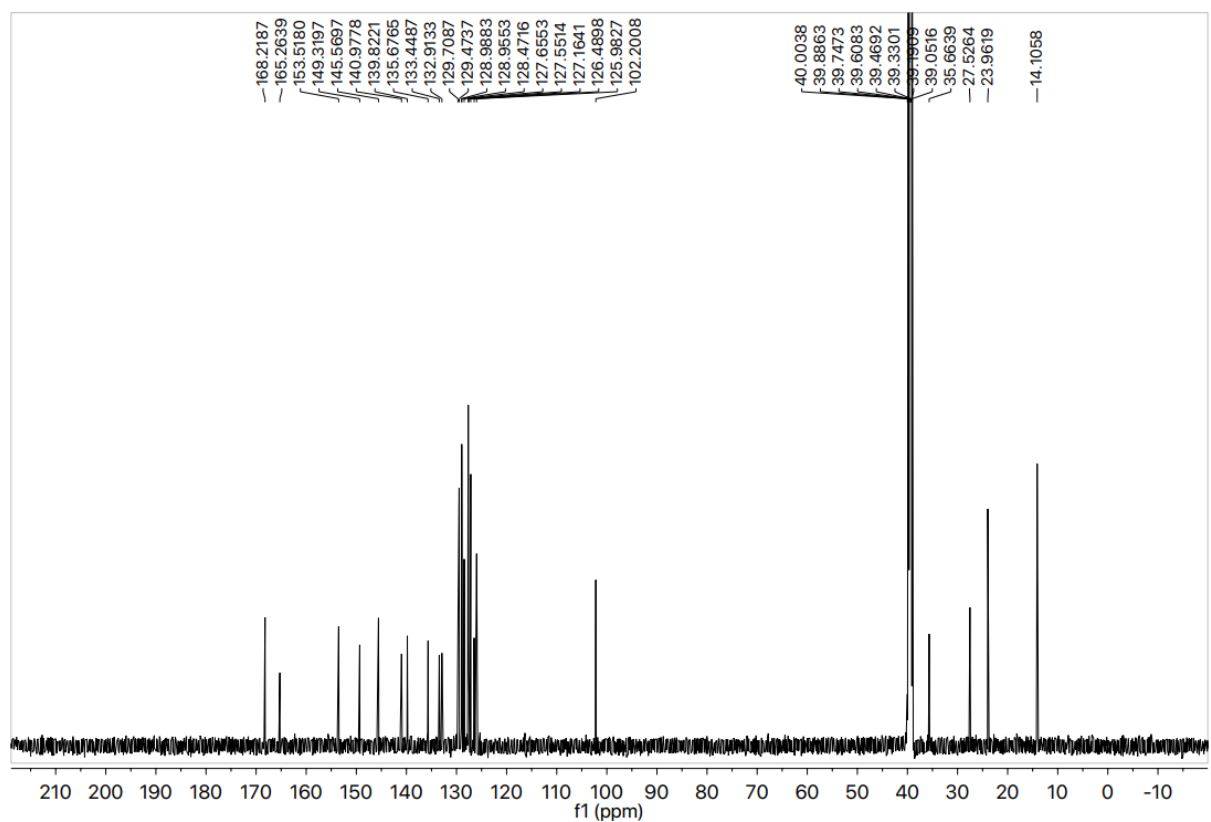


FIGURE S18 <sup>13</sup>C-NMR spectrum of **9j**

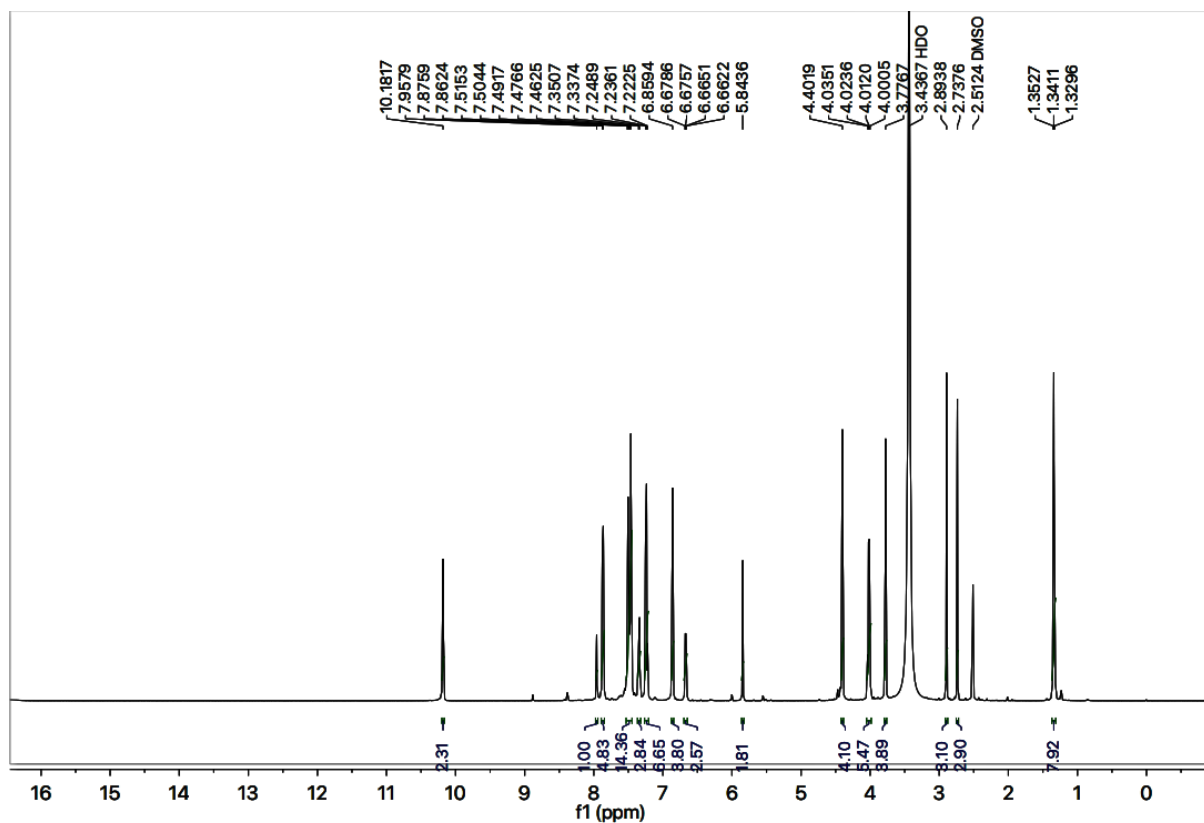


FIGURE S19  $^1\text{H-NMR}$  spectrum of **9k**

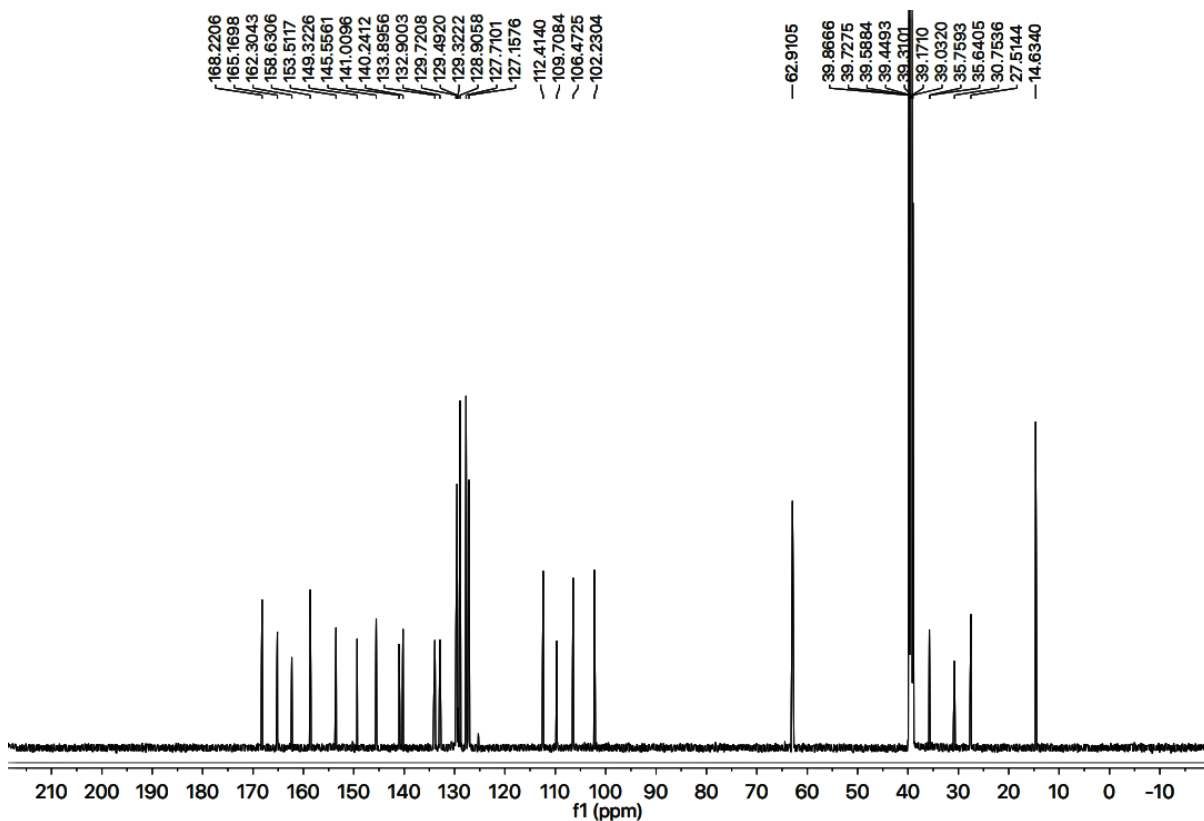
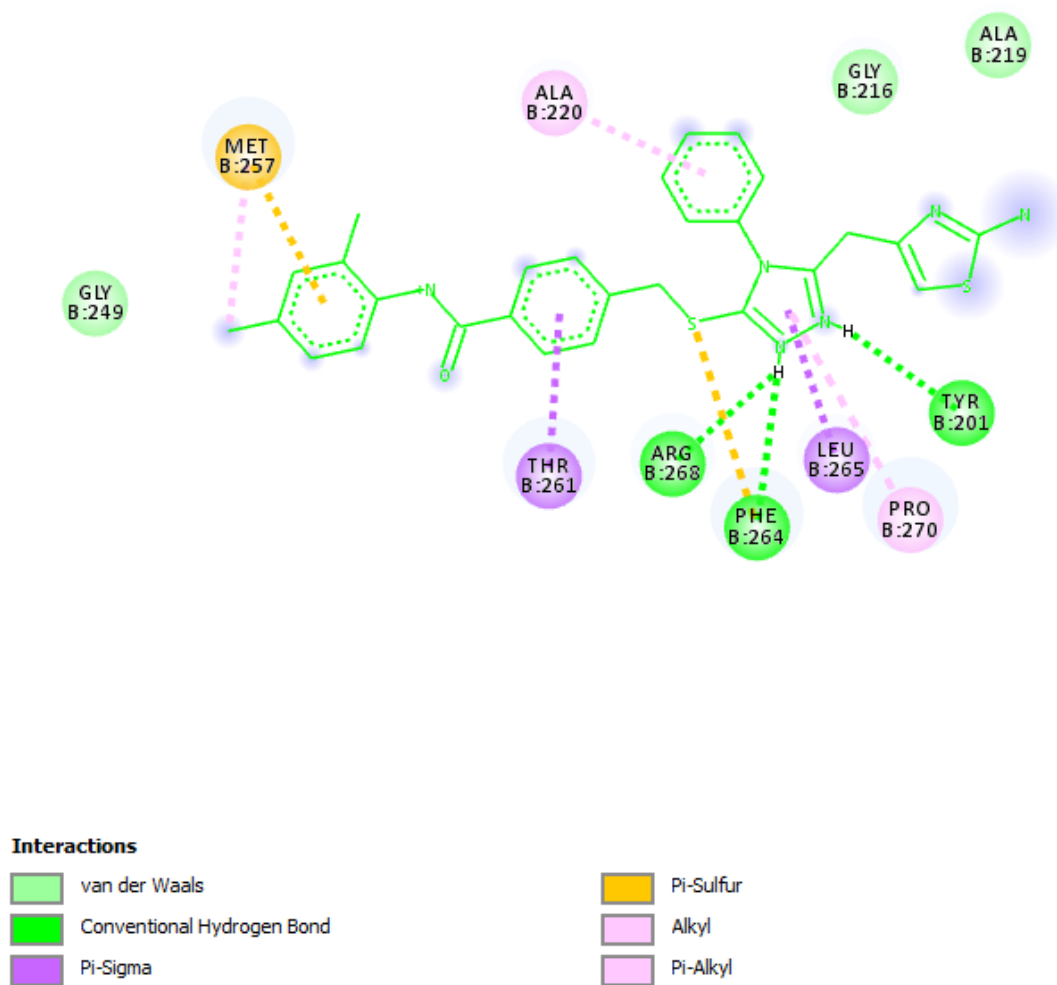
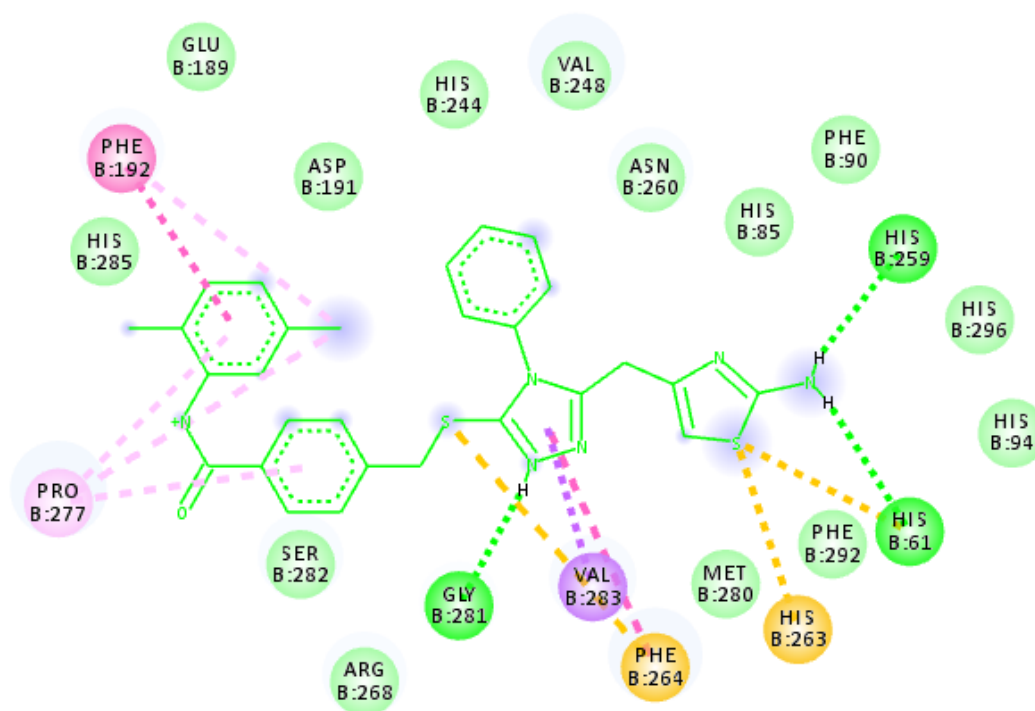





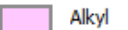

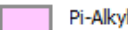

FIGURE S20  $^{13}\text{C-NMR}$  spectrum of **9k**



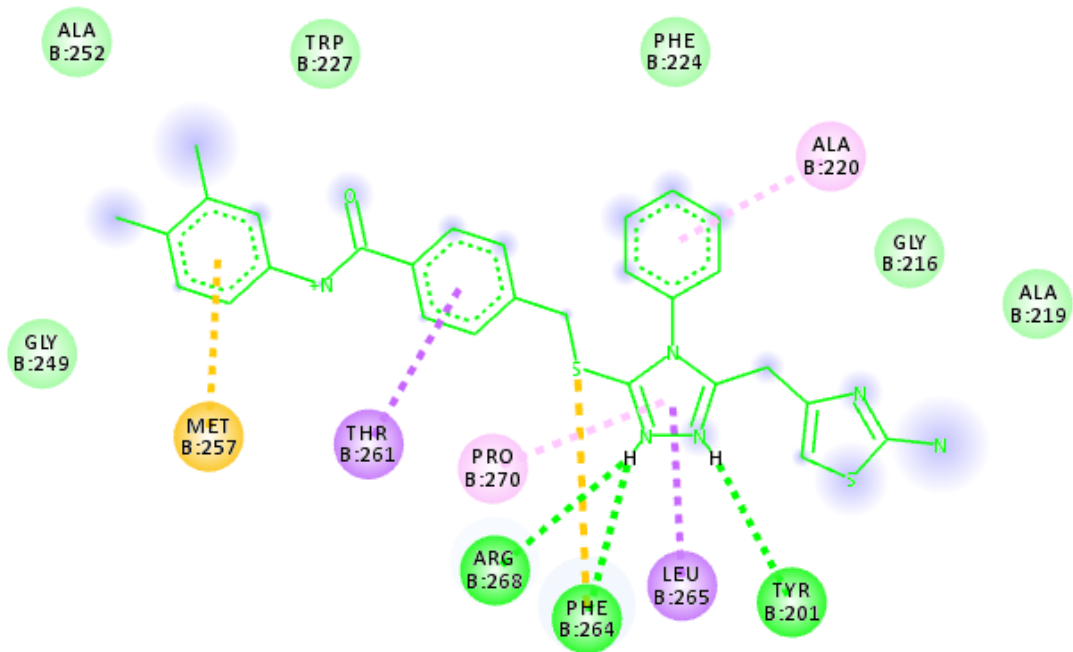
**FIGURE S21** Docked configuration of **9a**



**Interactions**

	van der Waals		Pi-Pi T-shaped
	Conventional Hydrogen Bond		Alkyl
	Pi-Sigma		Pi-Alkyl
	Pi-Sulfur		

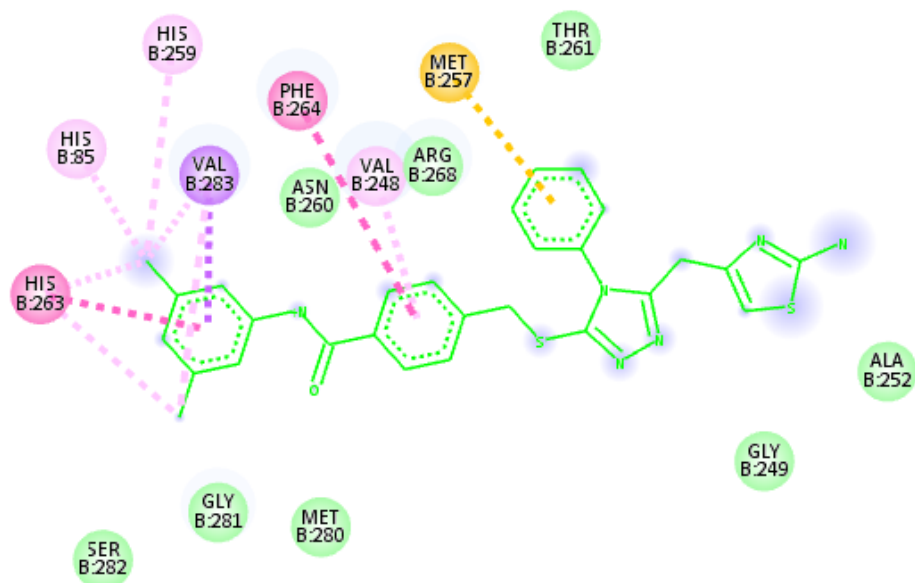
**FIGURE S22** Docked configuration of **9b**



**Interactions**

<span style="display: inline-block; width: 15px; height: 10px; background-color: #d9ead3; border: 1px solid #ccc; margin-right: 5px;"></span> van der Waals	<span style="display: inline-block; width: 15px; height: 10px; background-color: #f1c40f; border: 1px solid #ccc; margin-right: 5px;"></span> Pi-Sulfur
<span style="display: inline-block; width: 15px; height: 10px; background-color: #e74c3c; border: 1px solid #ccc; margin-right: 5px;"></span> Conventional Hydrogen Bond	<span style="display: inline-block; width: 15px; height: 10px; background-color: #fff3cd; border: 1px solid #ccc; margin-right: 5px;"></span> Pi-Alkyl
<span style="display: inline-block; width: 15px; height: 10px; background-color: #2980b9; border: 1px solid #ccc; margin-right: 5px;"></span> Pi-Sigma	

**FIGURE S23** Docked configuration of **9d**

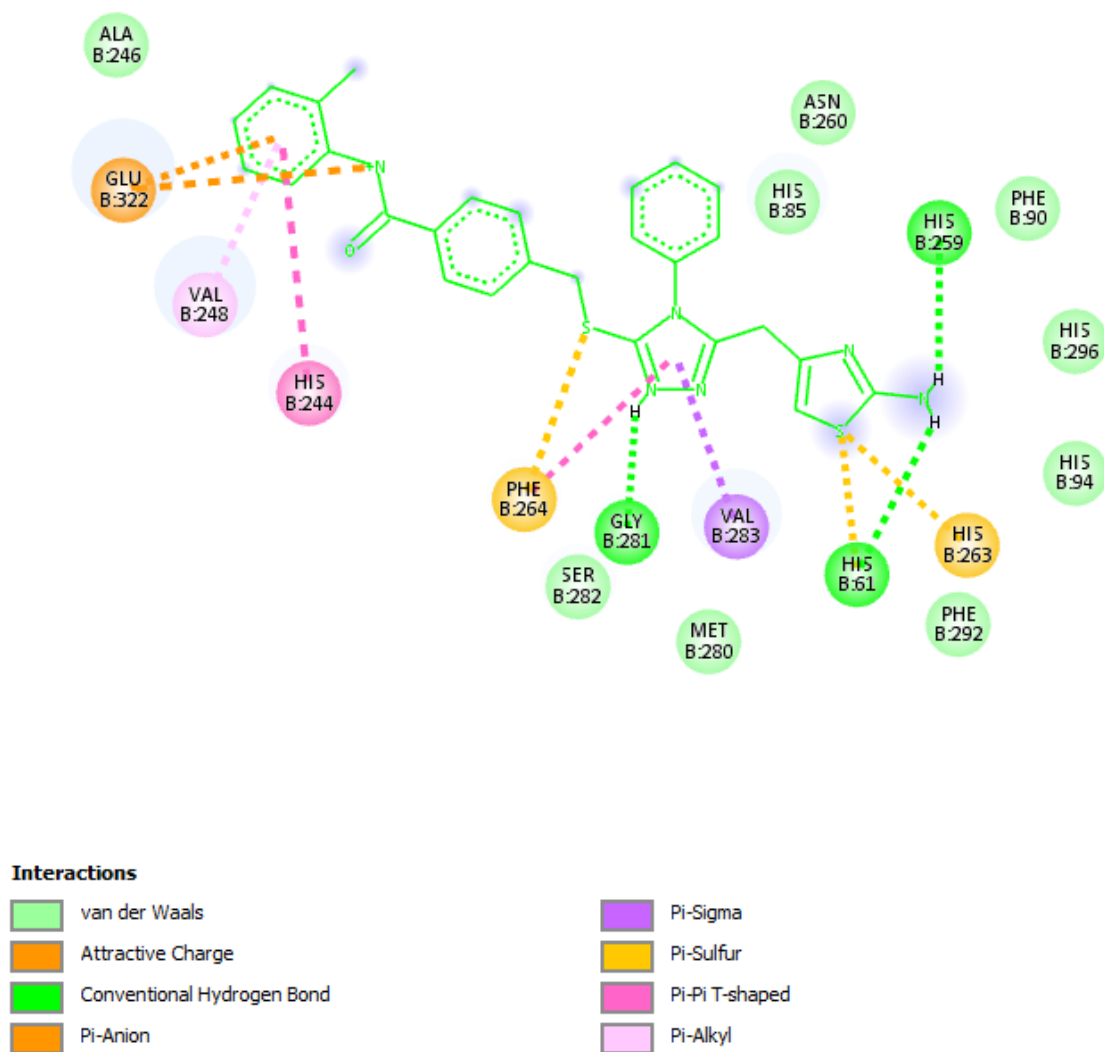


**Interactions**

- van der Waals
- Pi-Sigma
- Pi-Sulfur
- Pi-Pi Stacked

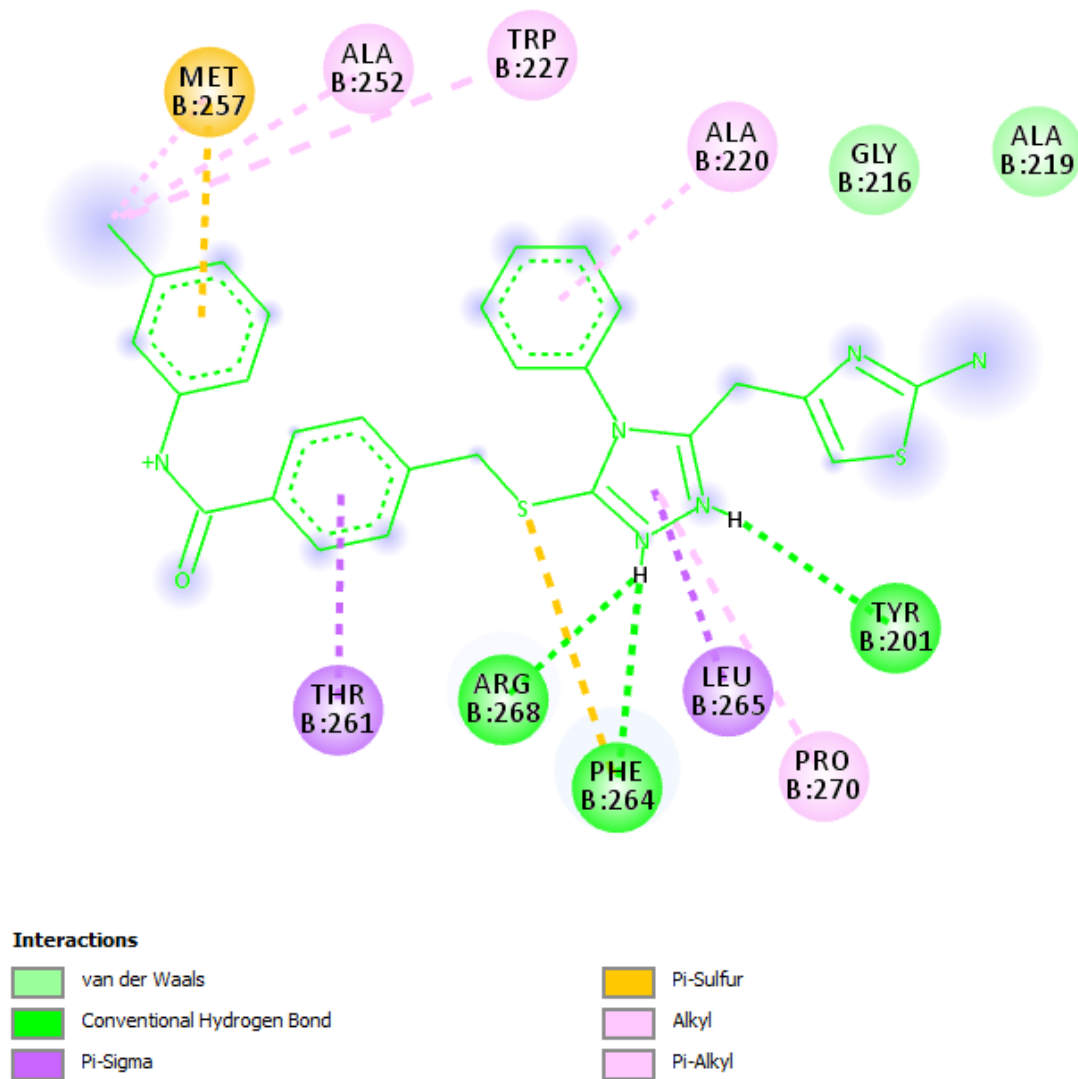
- Pi-Pi T-shaped
- Alkyl
- Pi-Alkyl

**FIGURE S24** Docked configuration of **9e**

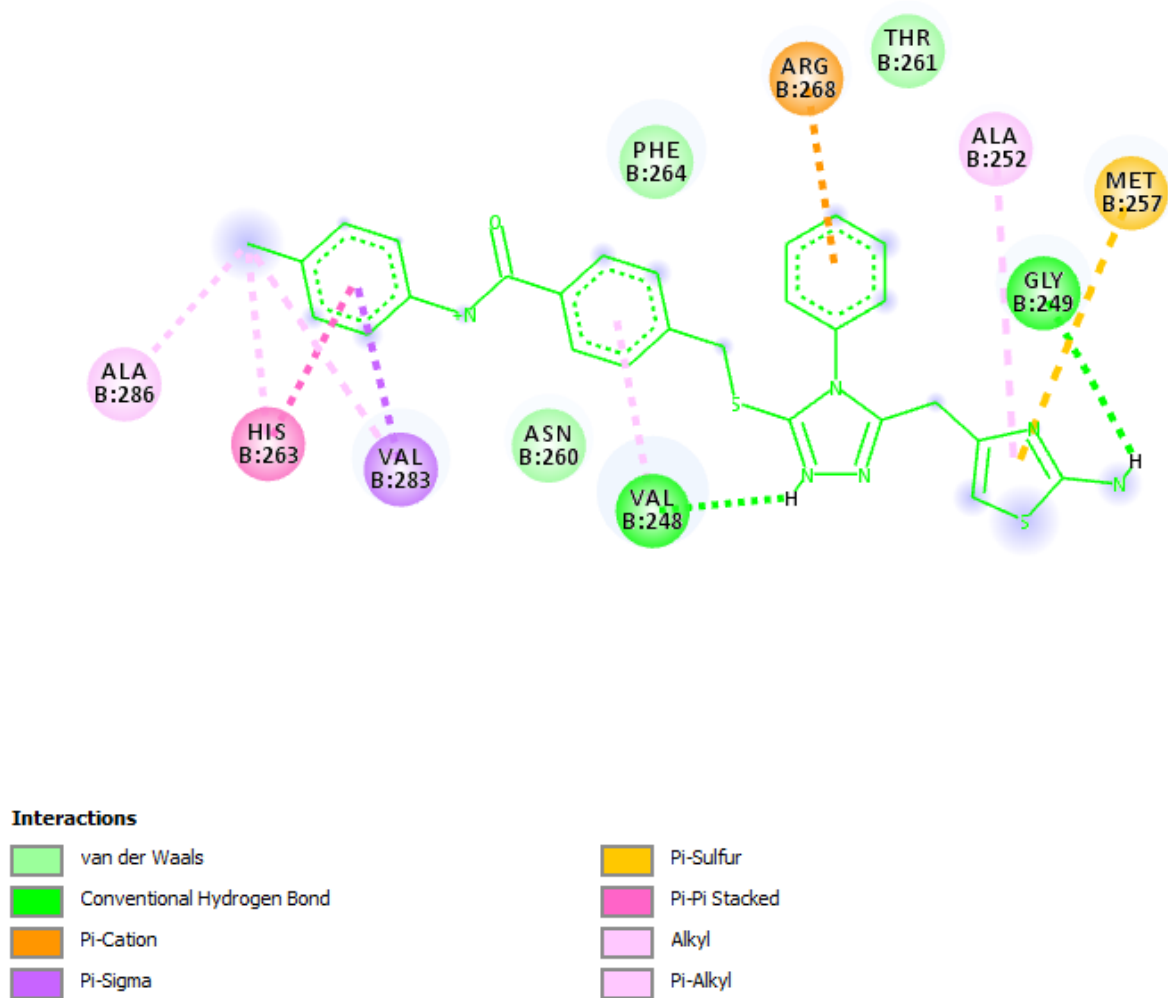


**FIGURE S25** Docked configuration of **9f**

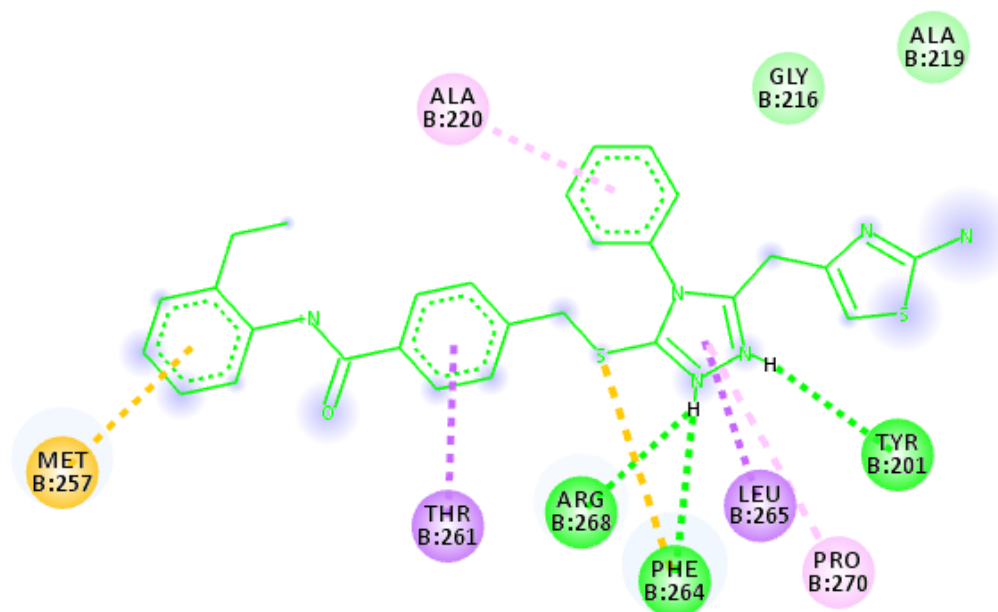




**FIGURE S26** Docked configuration of **9g**



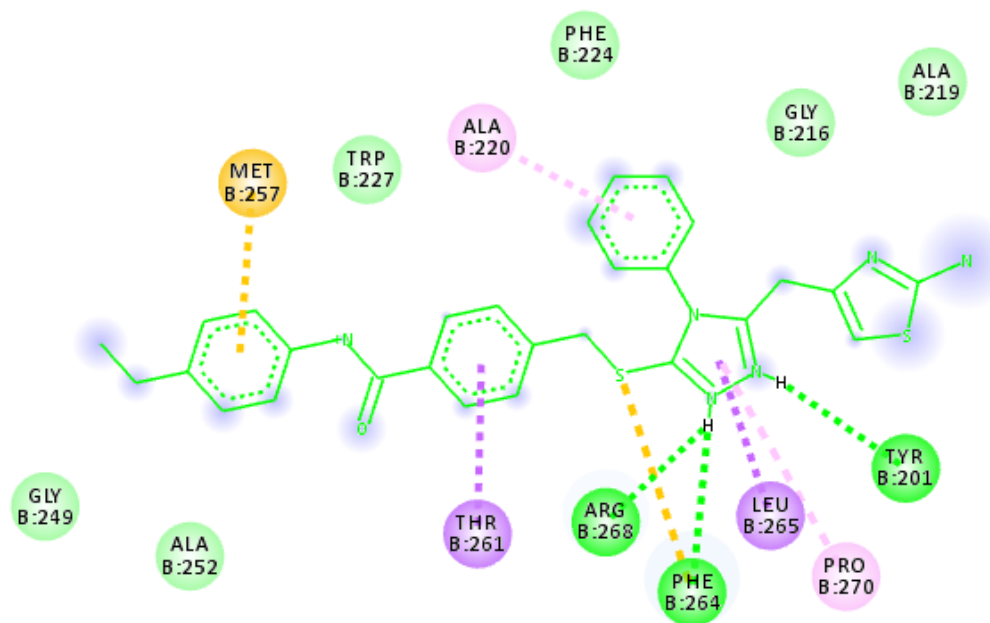
**FIGURE S27** Docked configuration of **9h**



**Interactions**

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<span style="display: inline-block; width: 15px; height: 10px; background-color: #f4cccc; border: 1px solid #ccc; margin-right: 5px;"></span> Conventional Hydrogen Bond	<span style="display: inline-block; width: 15px; height: 10px; background-color: #fff2cc; border: 1px solid #ccc; margin-right: 5px;"></span> Pi-Alkyl
<span style="display: inline-block; width: 15px; height: 10px; background-color: #d9ead3; border: 1px solid #ccc; margin-right: 5px;"></span> Pi-Sigma	

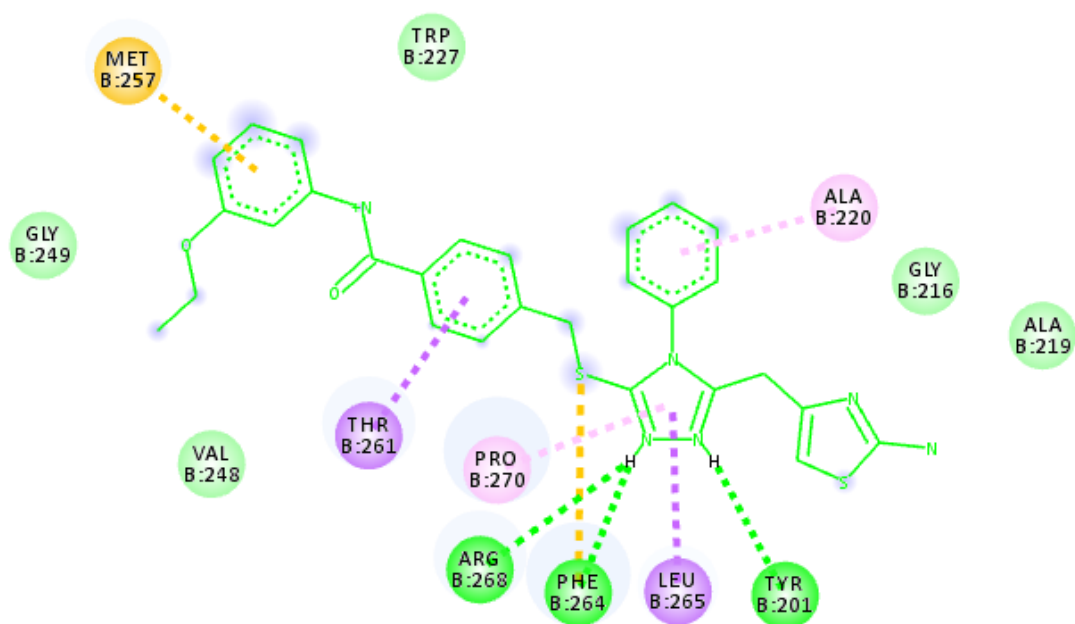
**FIGURE S28** Docked configuration of **9i**








**Interactions**

- |  |   |
|--|---|
| <span style="display: inline-block; width: 15px; height: 10px; background-color: #d9ead3; border: 1px solid #ccc; margin-right: 5px;"></span> van der Waals              | <span style="display: inline-block; width: 15px; height: 10px; background-color: #f1c40f; border: 1px solid #ccc; margin-right: 5px;"></span> Pi-Sulfur |
| <span style="display: inline-block; width: 15px; height: 10px; background-color: #27ae60; border: 1px solid #ccc; margin-right: 5px;"></span> Conventional Hydrogen Bond | <span style="display: inline-block; width: 15px; height: 10px; background-color: #f080f0; border: 1px solid #ccc; margin-right: 5px;"></span> Pi-Alkyl  |
| <span style="display: inline-block; width: 15px; height: 10px; background-color: #9b59b6; border: 1px solid #ccc; margin-right: 5px;"></span> Pi-Sigma                   |   |

**FIGURE S29** Docked configuration of **9j**



**Interactions**

	van der Waals		Pi-Sulfur
	Conventional Hydrogen Bond		Pi-Alkyl
	Pi-Sigma		

**FIGURE S30** Docked configuration of **9k**