

# Design, Synthesis, Molecular Docking, and Biological Evaluation of Pyrazole Hybrid Chalcone Conjugates as Potential Anticancer Agents and Tubulin Polymerization Inhibitors

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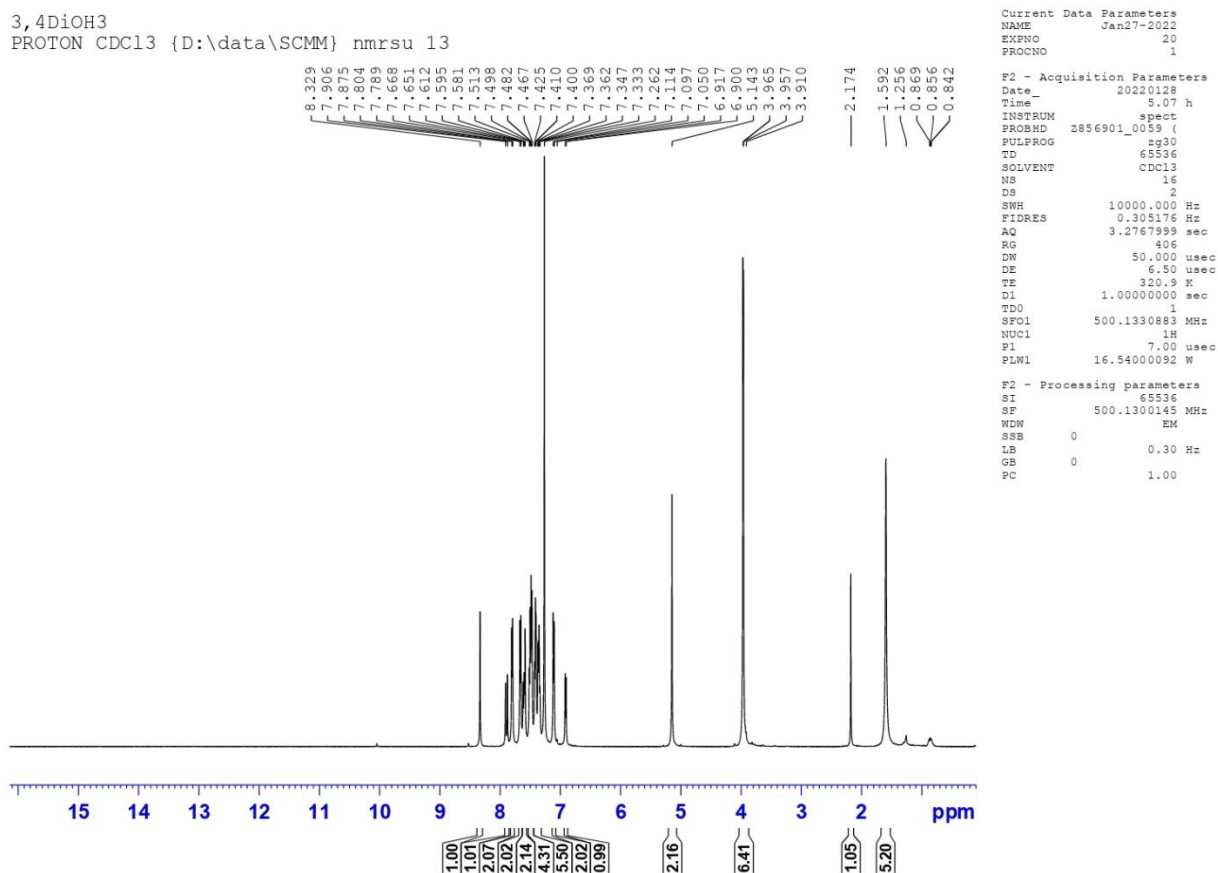
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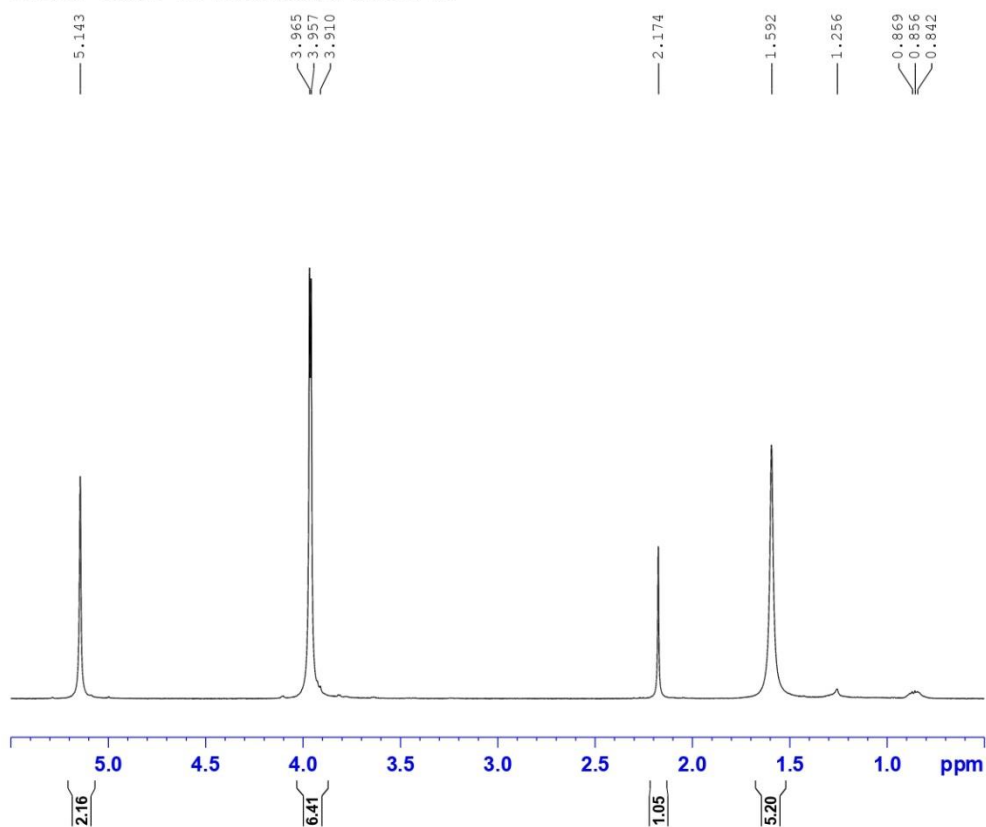
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**Figure S1.**  $^1\text{H}$  NMR of (E)-3-(3-(4-(benzyloxy)phenyl)-1-phenyl-1H-pyrazol-4-yl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one.

3,4DiOH3  
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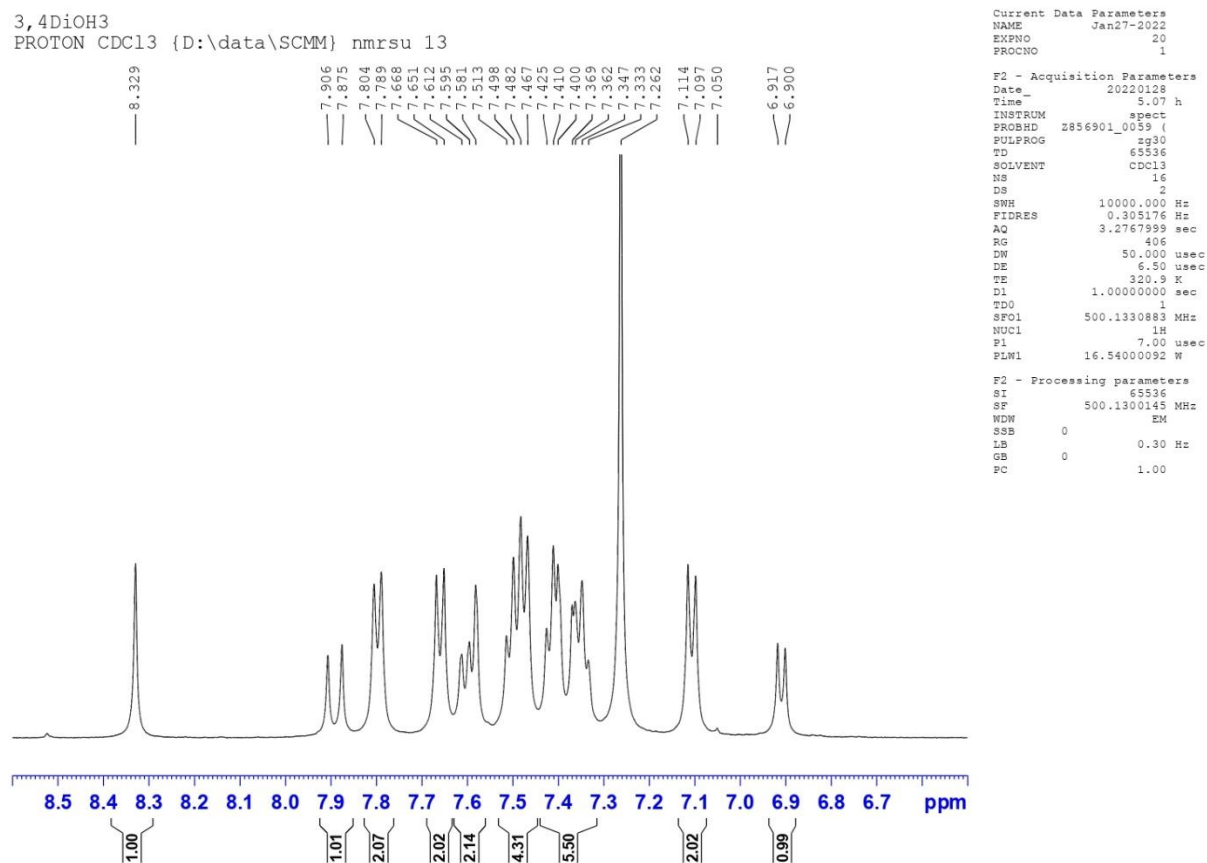


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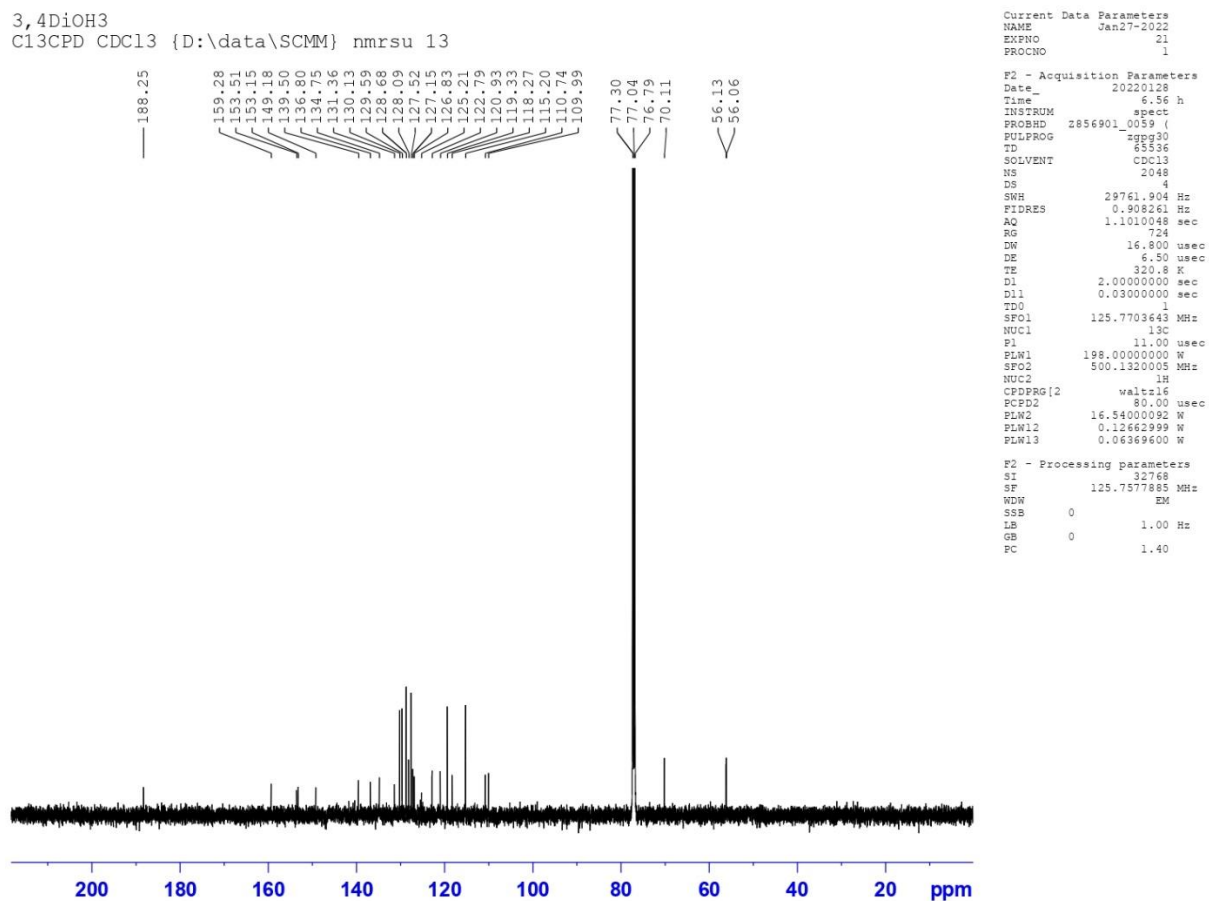
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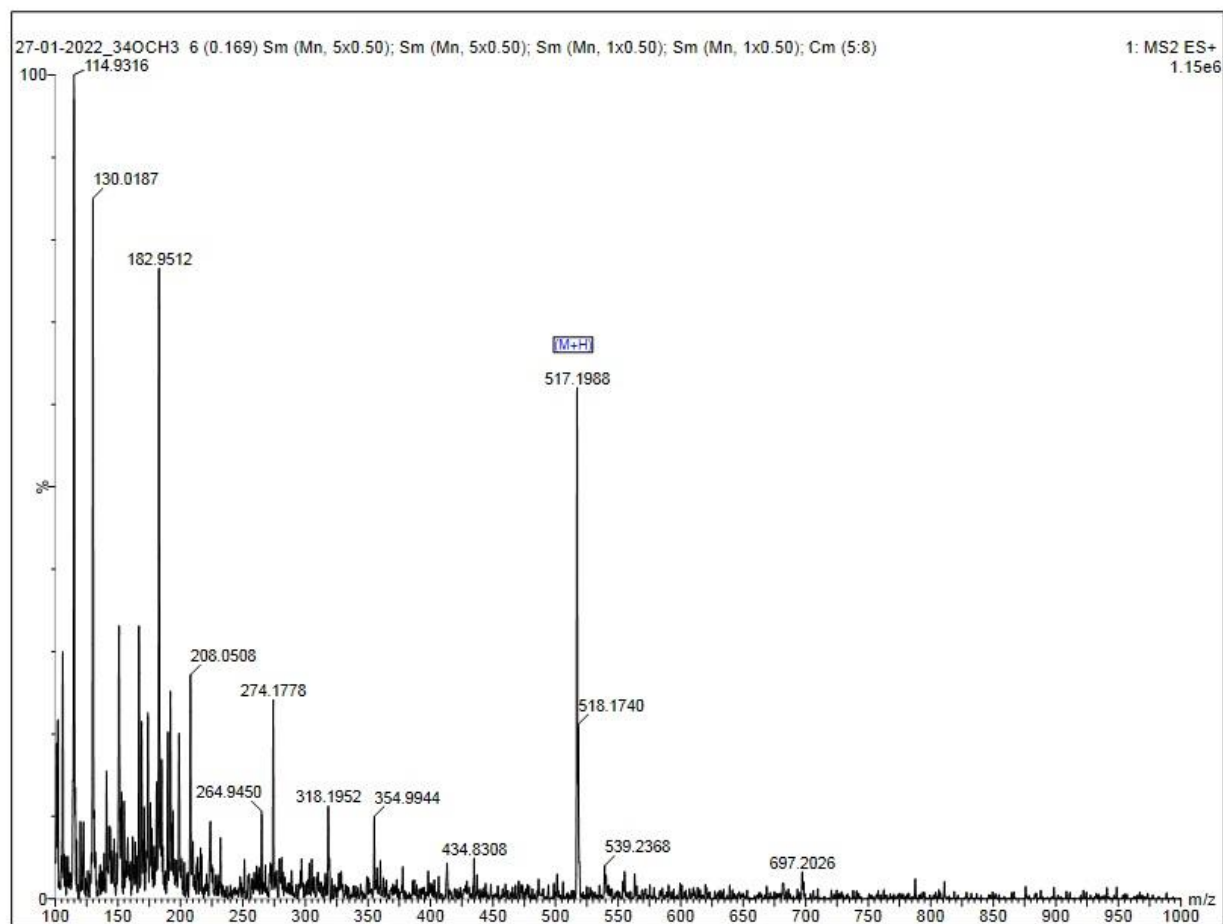
**Figure S2.**  $^{13}\text{C}$  NMR of (E)-3-(3-(4-(benzyloxy)phenyl)-1-phenyl-1H-pyrazol-4-yl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one.



**Figure S3.**  $^1\text{H}$  NMR of (E)-3-(3-(4-(benzyloxy)phenyl)-1-phenyl-1H-pyrazol-4-yl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one.

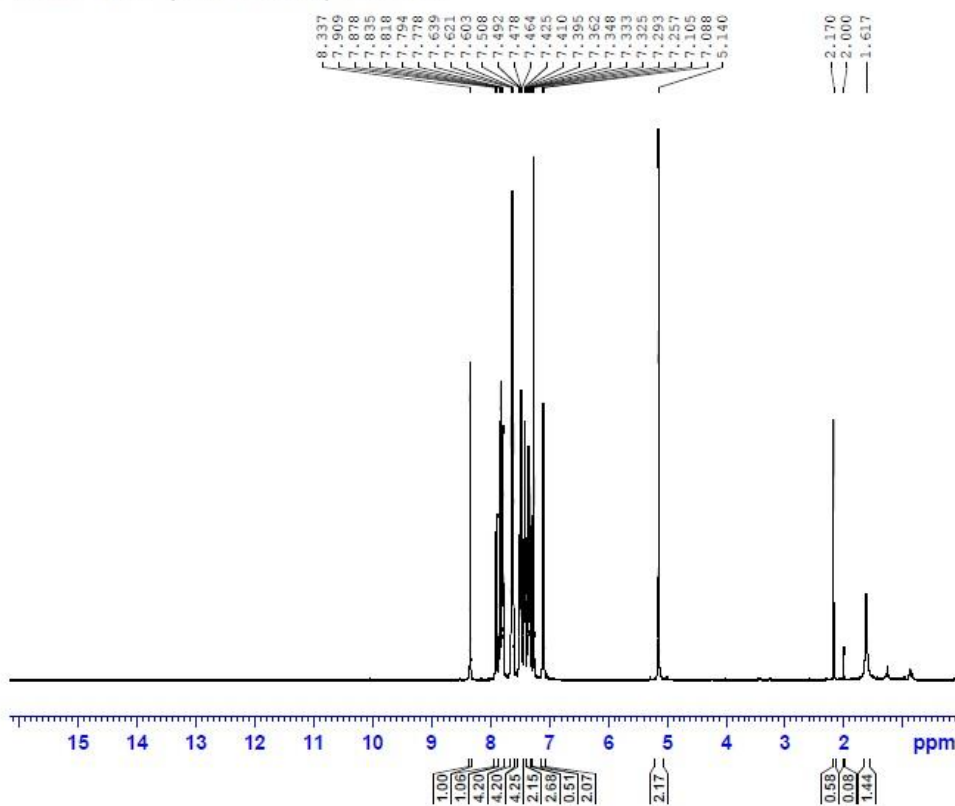


**Figure S4.**  $^{13}\text{C}$  NMR of (E)-3-(3-(4-(benzyloxy)phenyl)-1-phenyl-1H-pyrazol-4-yl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one.



**Figure S5.** Mass spectra of (E)-3-(3-(4-(benzyloxy)phenyl)-1-phenyl-1H-pyrazol-4-yl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one.

4-Br  
 PROTON CDCl3 {D:\data\SCMM} nmrsu 15



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Figure S6. <sup>1</sup>H NMR of (E)-3-(3-(4-(benzyloxy)phenyl)-1-phenyl-1H-pyrazol-4-yl)-1-(4-bromophenyl)prop-2-en-1-one.

4-Br  
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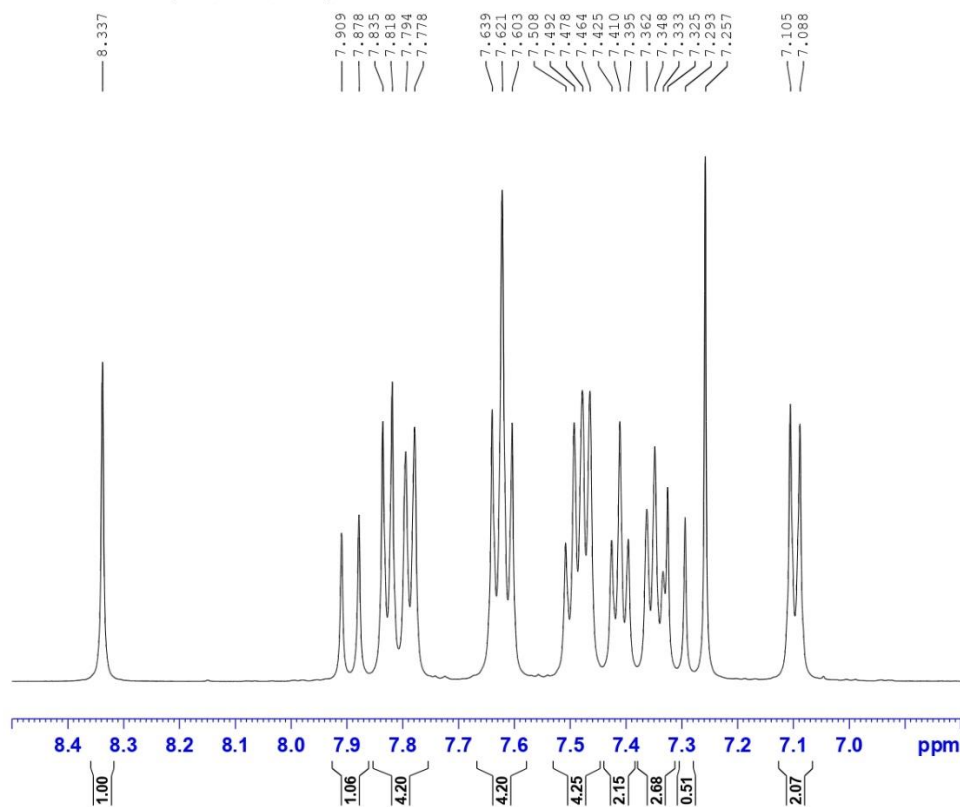
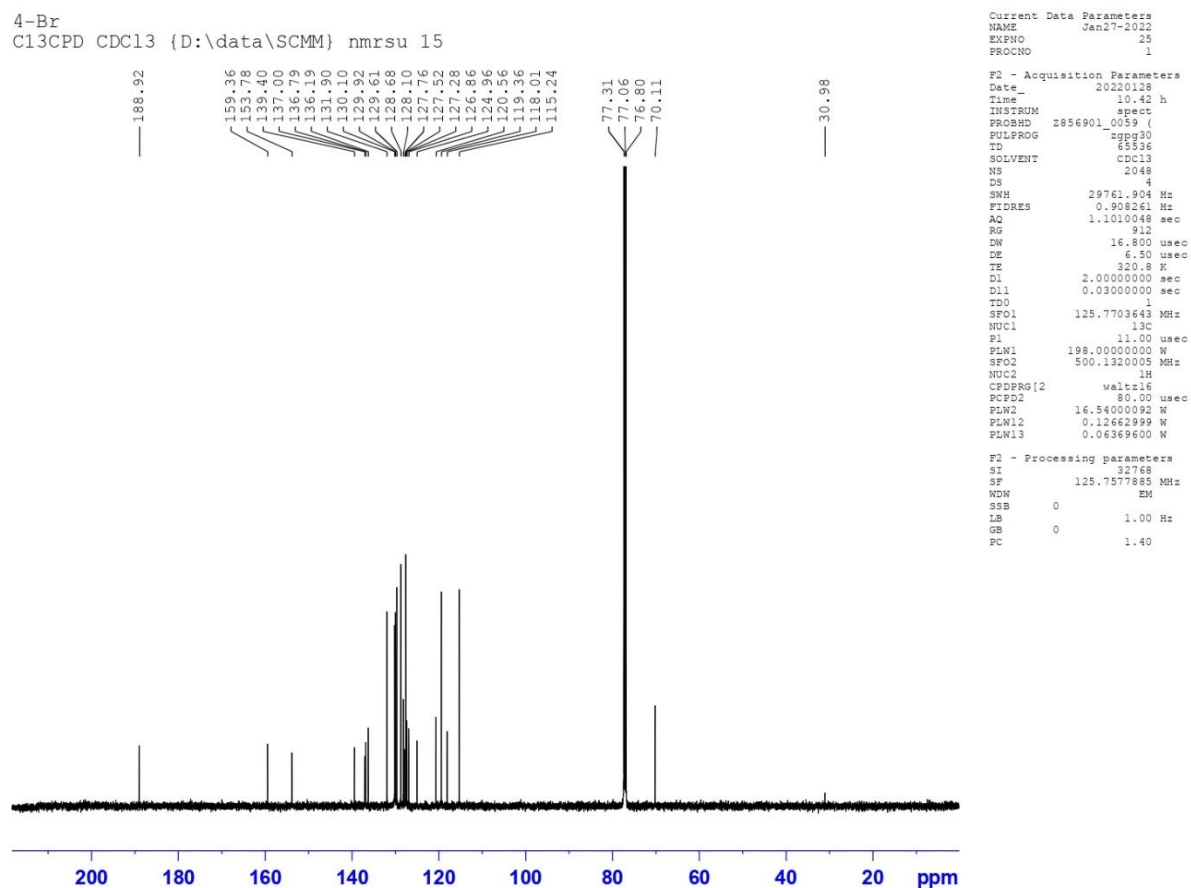
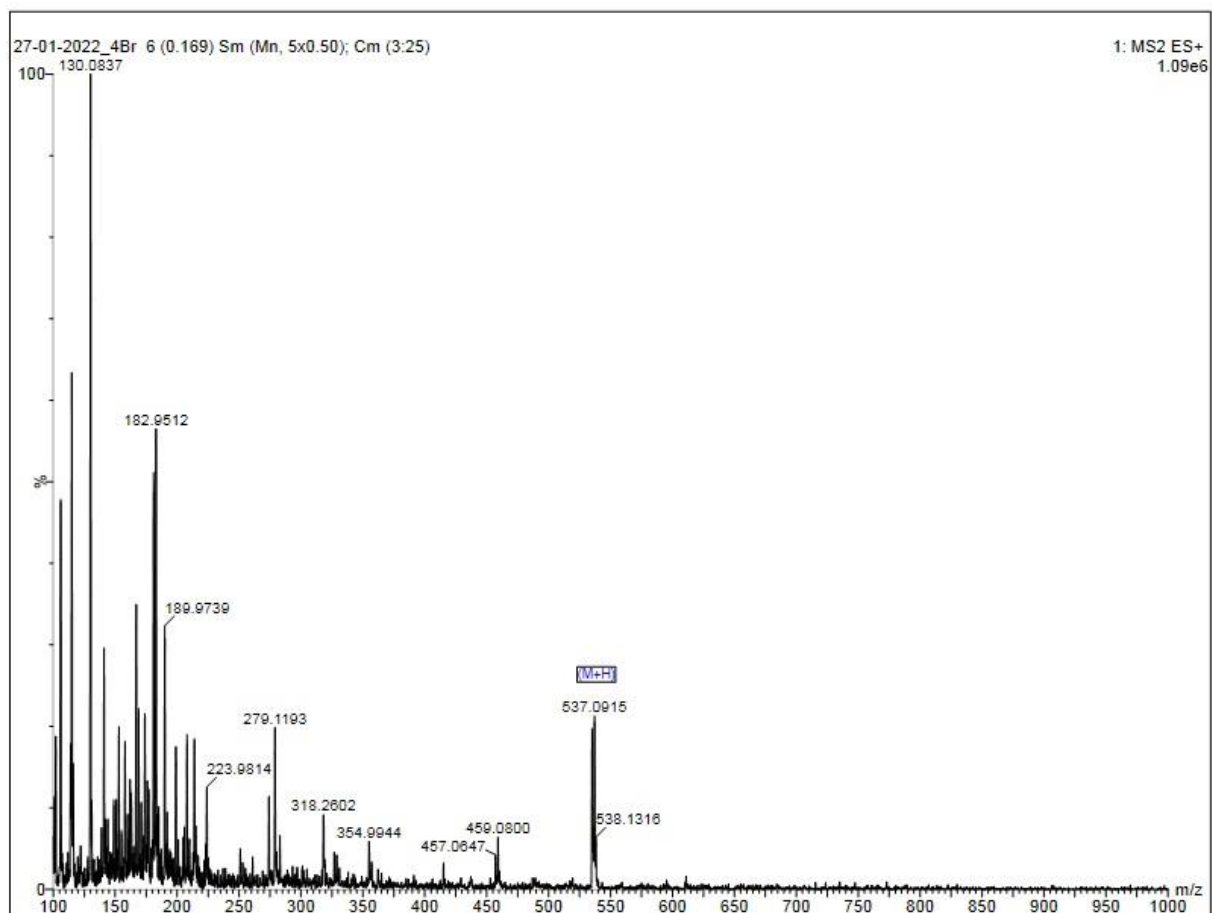


Figure S7. <sup>1</sup>H NMR of (E)-3-(3-(4-(benzyloxy)phenyl)-1-phenyl-1H-pyrazol-4-yl)-1-(4-bromophenyl)prop-2-en-1-one.

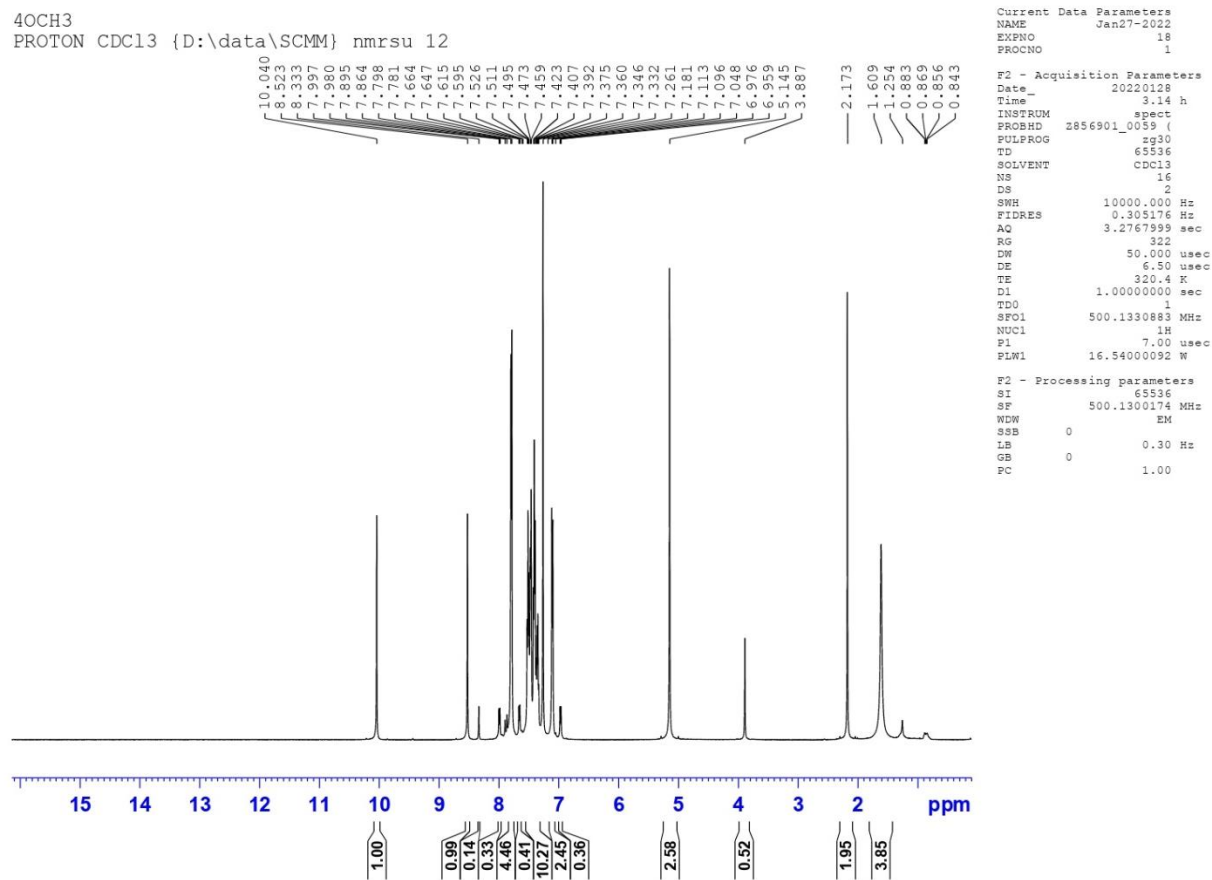




**Figure S8.**  $^{13}\text{C}$  NMR of (E)-3-(3-(4-(benzyloxy)phenyl)-1-phenyl-1H-pyrazol-4-yl)-1-(4-bromophenyl)prop-2-en-1-one.

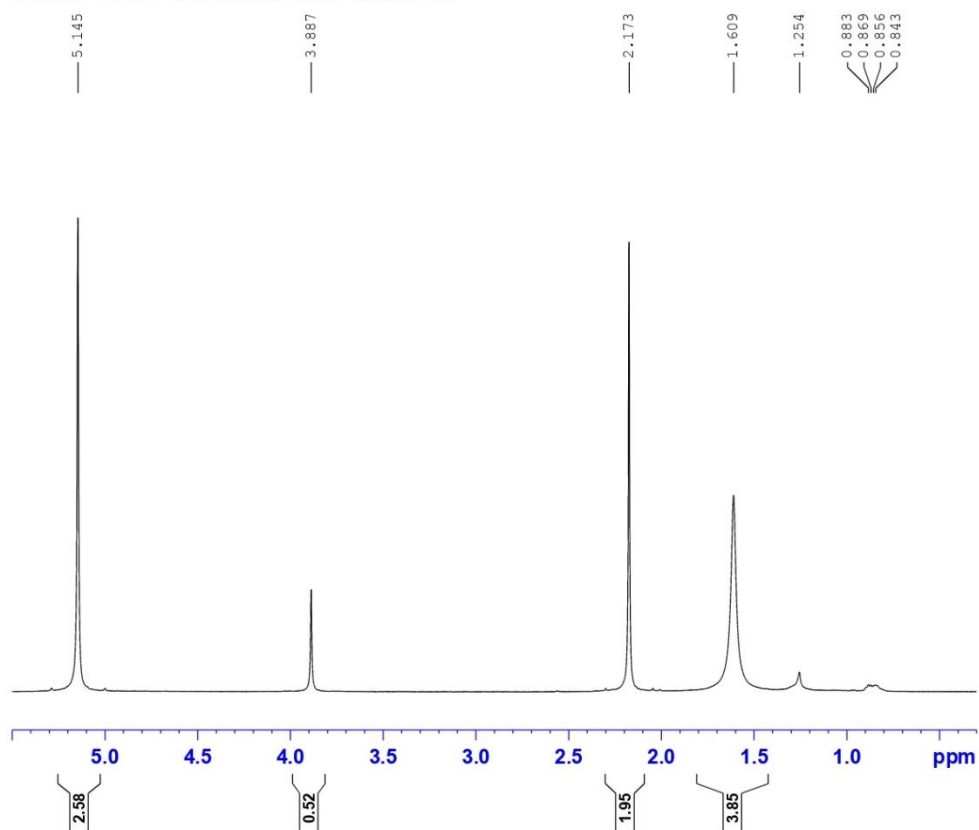


**Figure S9.** Mass spectra of (E)-3-(3-(4-(benzyloxy)phenyl)-1-phenyl-1H-pyrazol-4-yl)-1-(4-bromophenyl)prop-2-en-1-one.



**Figure S10.**  $^1\text{H}$  NMR of (E)-3-(3-(4-(benzyloxy)phenyl)-1-phenyl-1H-pyrazol-4-yl)-1-(4-methoxyphenyl)prop-2-en-1-one.

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PROTON CDC13 {D:\data\SCMM} nmrsu 12

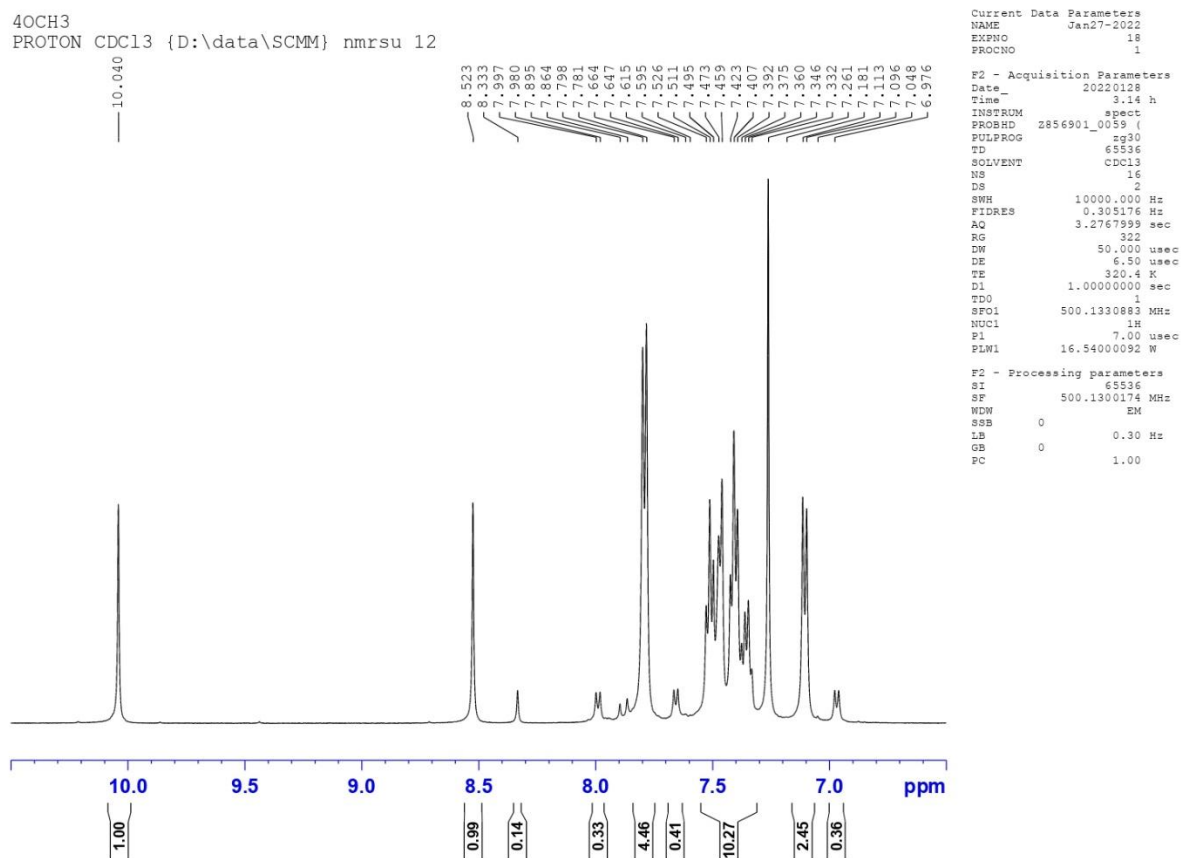


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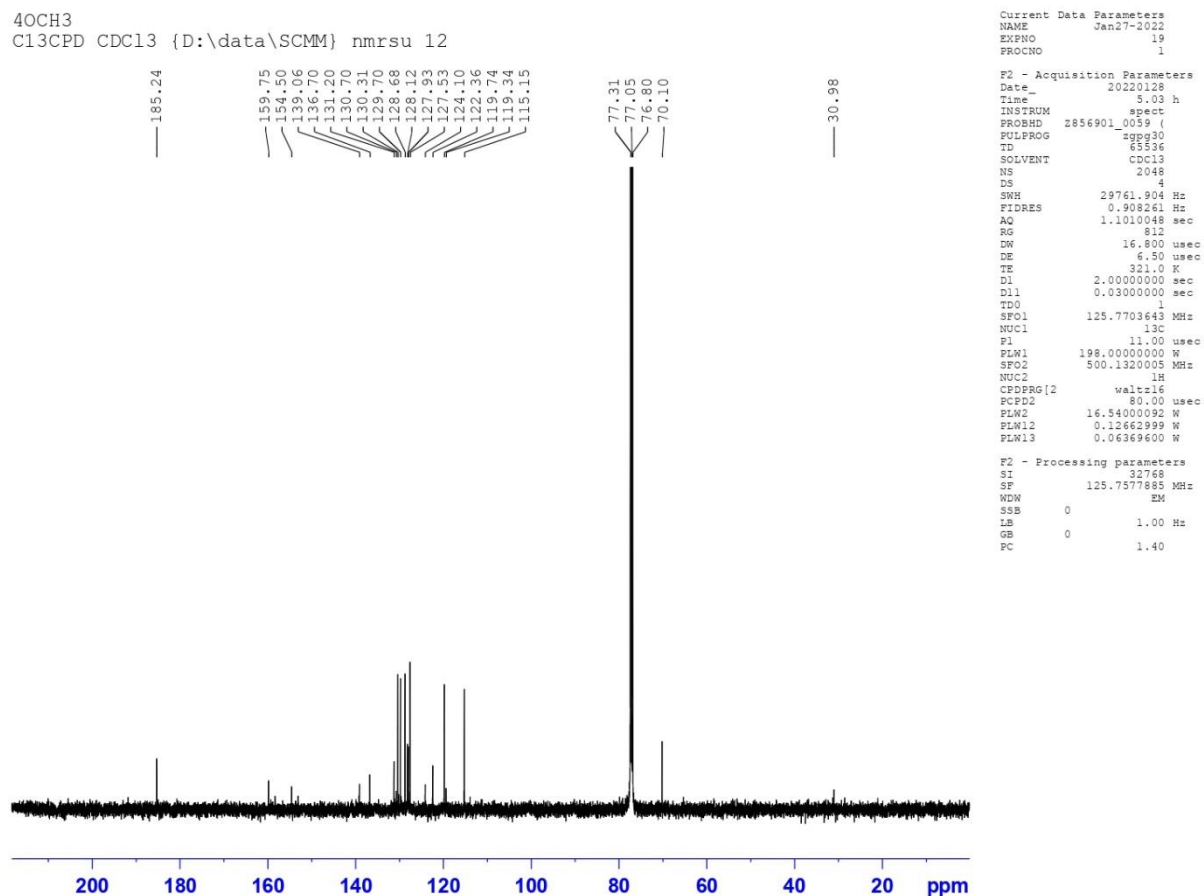
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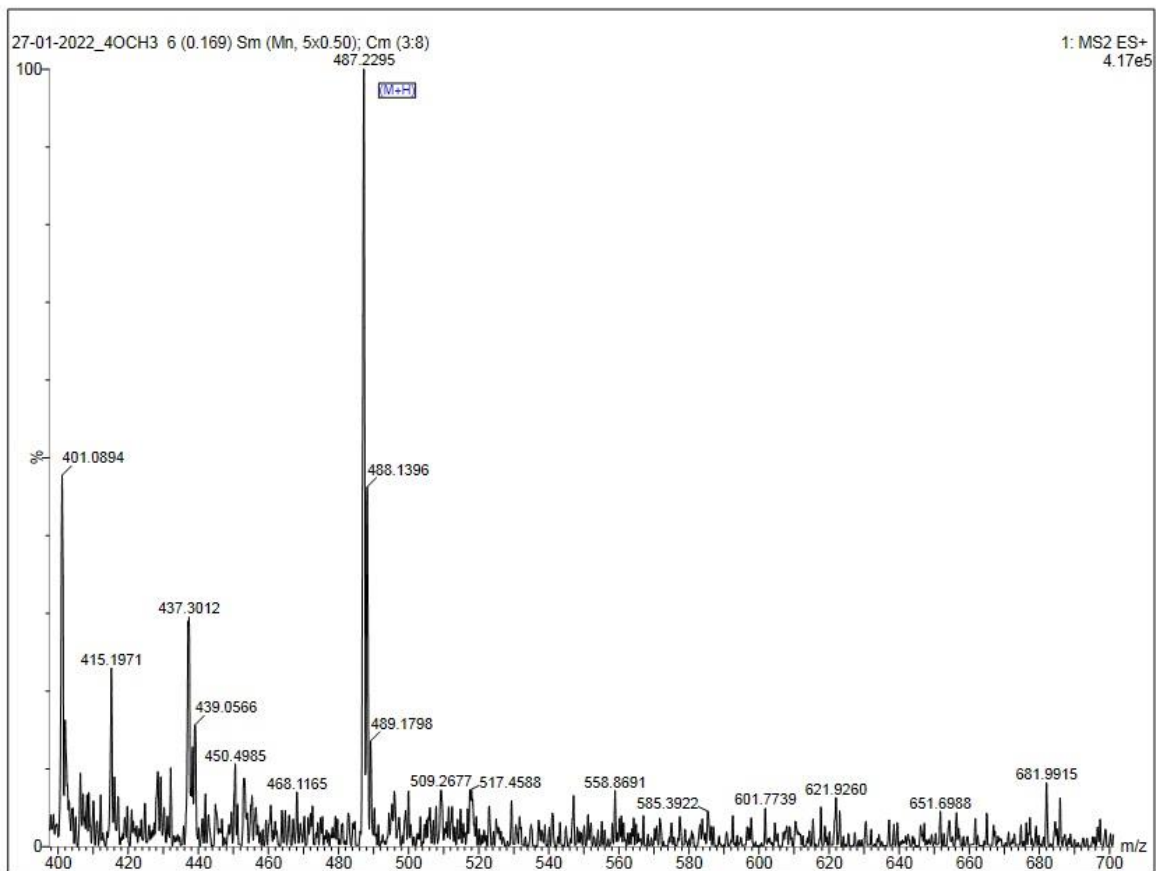
**Figure S11.**  $^1\text{H}$  NMR of (E)-3-(3-(4-(benzyloxy)phenyl)-1-phenyl-1H-pyrazol-4-yl)-1-(4-methoxyphenyl)prop-2-en-1-one.



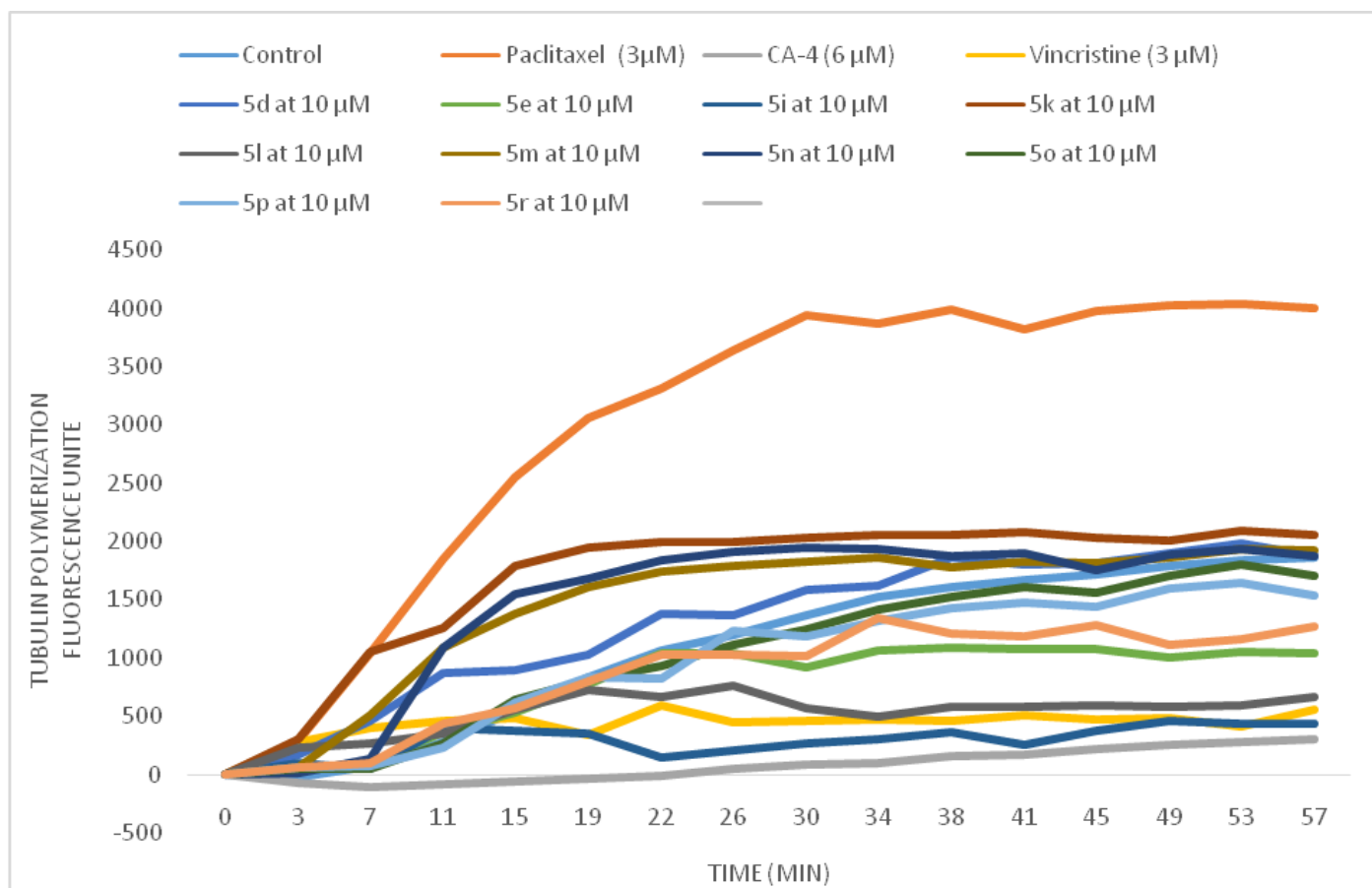
**Figure S12.**  $^1\text{H}$  NMR of (E)-3-(3-(4-(benzyloxy)phenyl)-1-phenyl-1H-pyrazol-4-yl)-1-(4-methoxyphenyl)prop-2-en-1-one.



**Figure S13.**  $^{13}\text{C}$  NMR of (E)-3-(3-(4-(benzyloxy)phenyl)-1-phenyl-1H-pyrazol-4-yl)-1-(4-methoxyphenyl)prop-2-en-1-one.



**Figure S14.** Mass spectra of (E)-3-(3-(4-(benzyloxy)phenyl)-1-phenyl-1H-pyrazol-4-yl)-1-(4-methoxyphenyl)prop-2-en-1-one.



**Figure S15.** Effect of lead conjugates **5d**, **5e**, **5i**, **5k**, **5l**, **5m**, **5n**, **5o**, **5p** and **5r** on tubulin polymerization: Tubulin polymerization was monitored by the increase in fluorescence at 360 nm (excitation) and 420 nm (emission) for 1 h at 37 °C. Combretastatin A-4 was used as the reference standard in this study.