International Journal of *Molecular Sciences*

MDPI

Supplementary material

Molecular docking and biophysical studies for antiproliferative assessment of synthetic pyrazolo-pyrimidinones tethered with hydrazide-hydrazones

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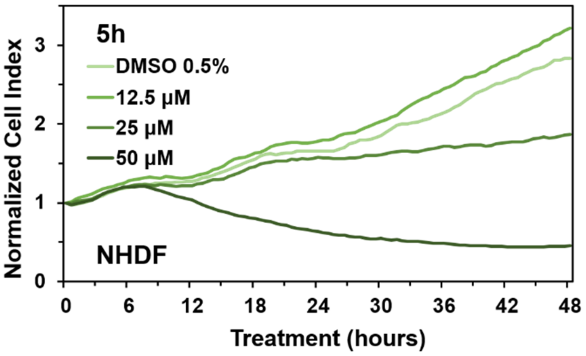

IC_{50} - NHDF

Compound	IC_{50} (μM) ± SE
5a	60.18 ± 2.908
5e	66.16 ± 3.367
5g	26.05 ± 1.110
5h	32.07 ± 1.703
CDDP	14.86 ± 0.802

Figure S1. Real time monitoring of NHDF cell viability after 48 h exposure to synthetic compounds **5a**, **5e**, **5g**, and **5h**, using the xCELLigence System Real-Time Cell Analyzer. Left panel, representative NCI traces of NHDF cells exposed to increasing concentrations (12.5, 25, 50 μM) of **5h** and 0.5% DMSO vehicle (control) for 48 hours. Right panel, IC_{50} values (± standard error, SE) of cisplatin (CDDP), **5a**, **5e**, **5g**, and **5h** against NHDF cells after 48h drug exposure. The IC_{50} value represents the concentration of each compound that reduces the NCI by 50%. Data are means of three independent experiments.

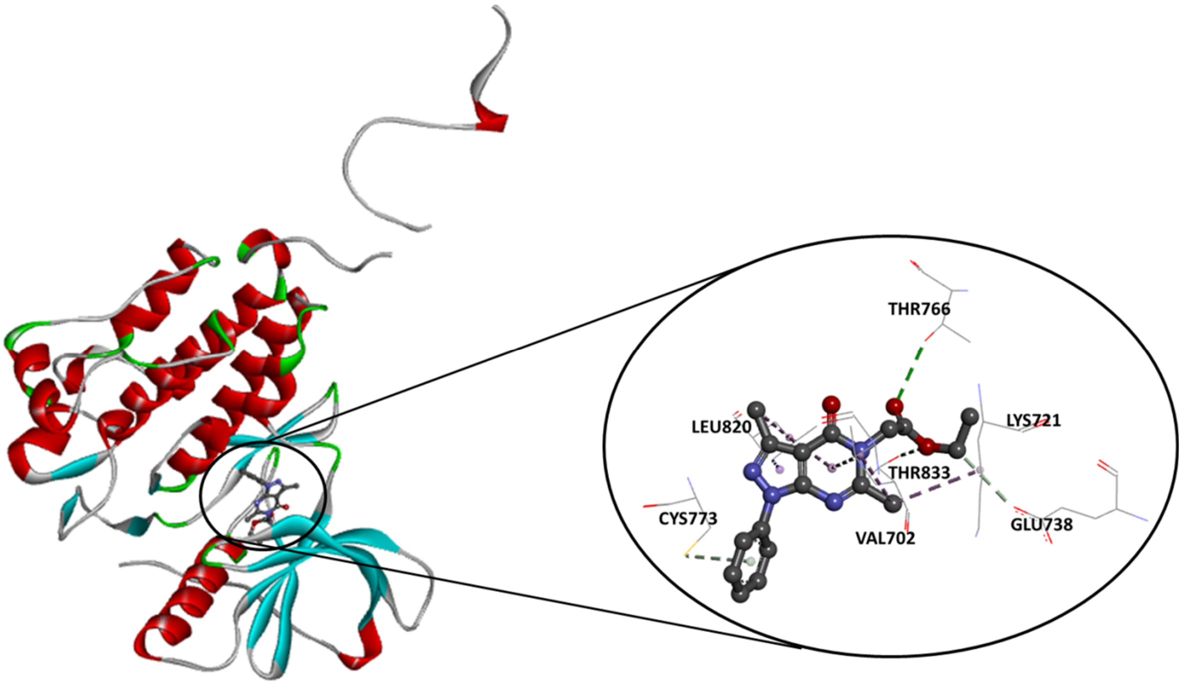

Figure S2. Binding mode of ester **3** in the Erlotinib binding site of EGFR (PDB:1M17).

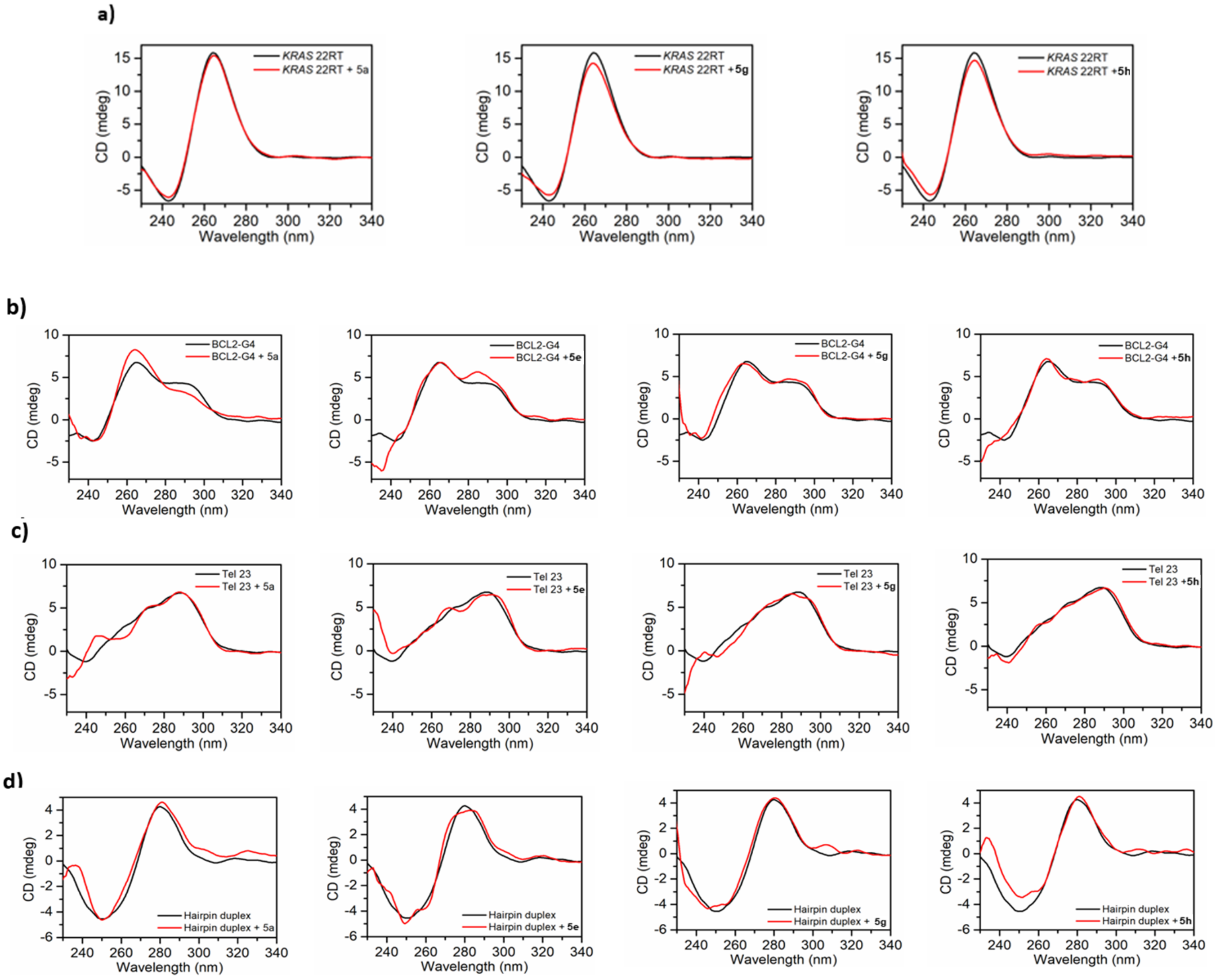

Figure S3. CD spectra of **a)** *KRAS* 22RT, **b)** BCL2-G4, **c)** Tel 23 and **d)** Hairpin duplex in the absence (black line) and in the presence (red line) of **5a**, **5e**, **5g** and **5h**.

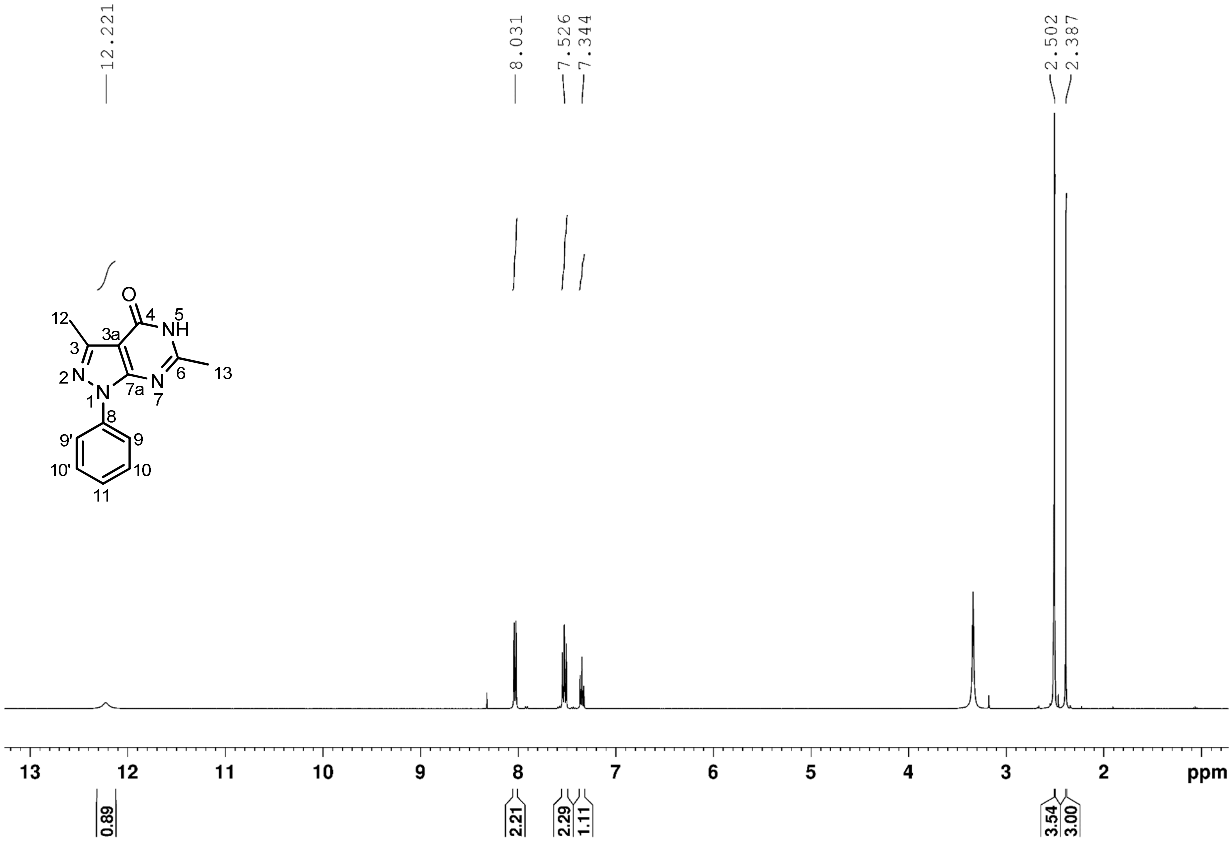

Figure S4. ^{1}H NMR spectrum of compound **2** (DMSO-*d*$_6$, 400MHz).

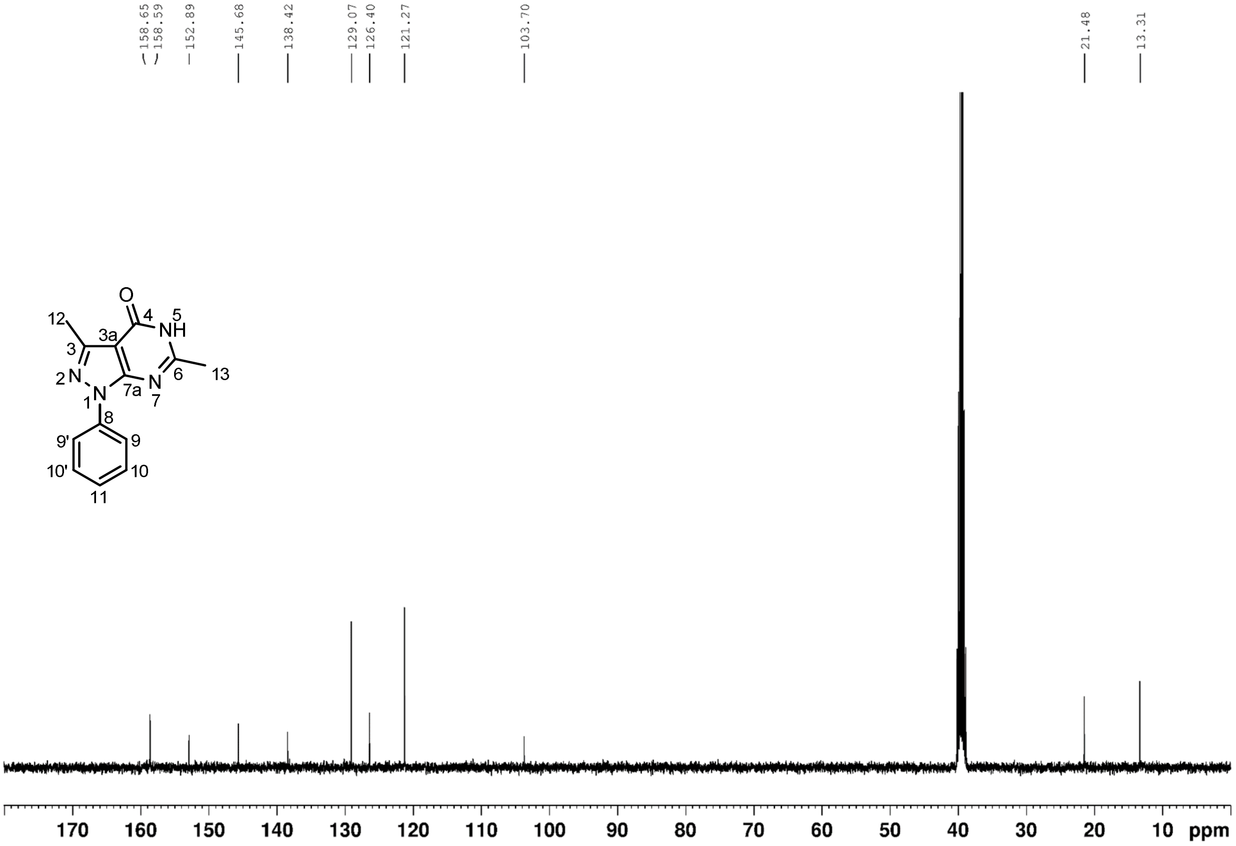

Figure S5. ^{13}C NMR spectrum of compound **2** (DMSO-*d*$_6$, 100MHz).

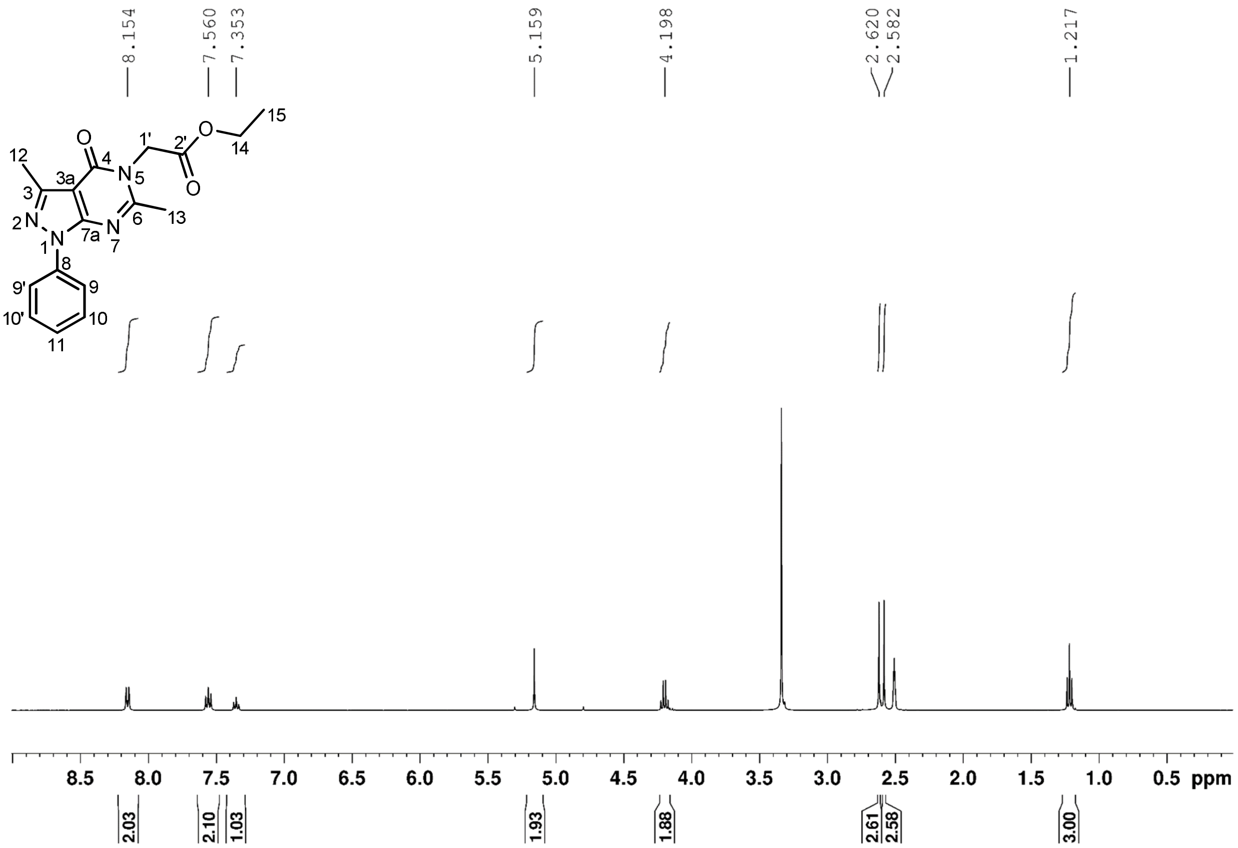

Figure S6. ^{1}H NMR spectrum of compound **3** (DMSO-d_6, 400MHz).

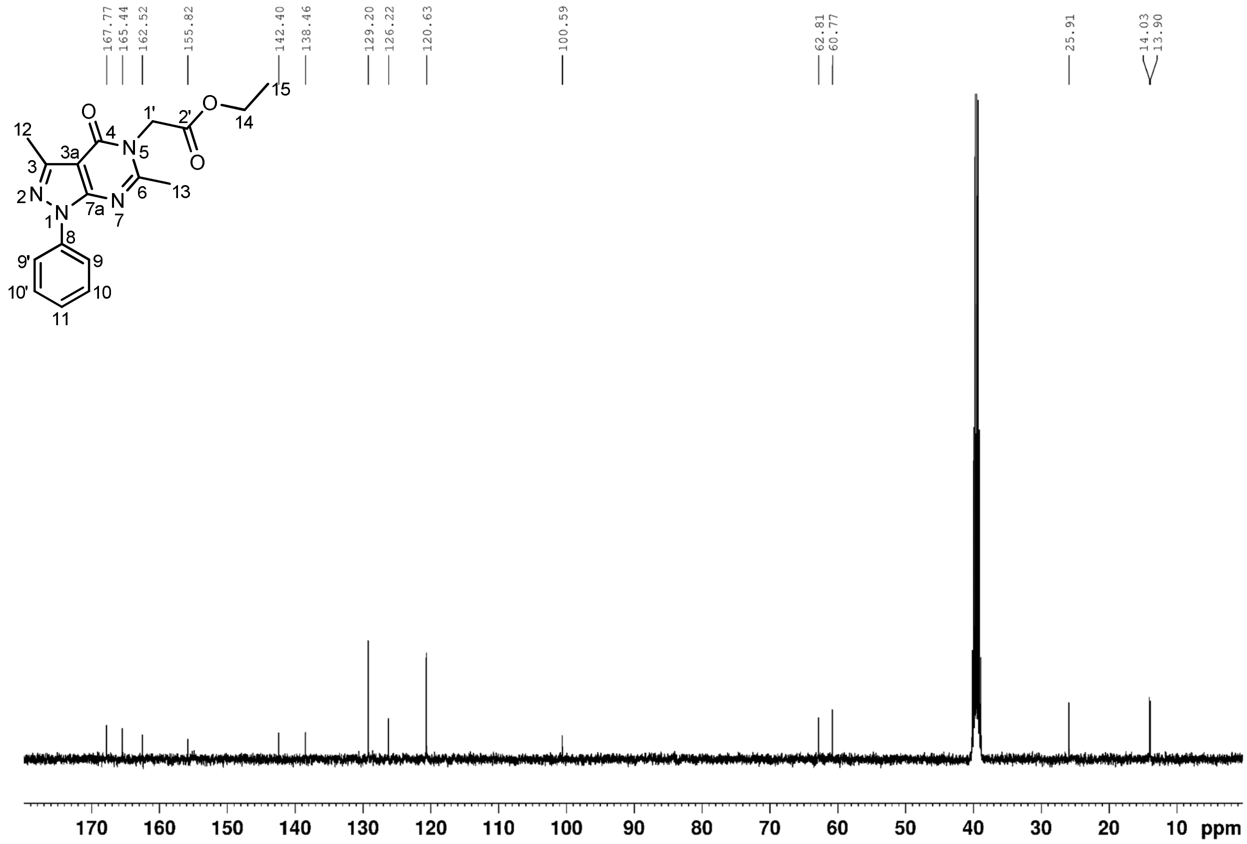

Figure S7. ^{13}C NMR spectrum of compound **3** (DMSO-d_6, 100MHz).

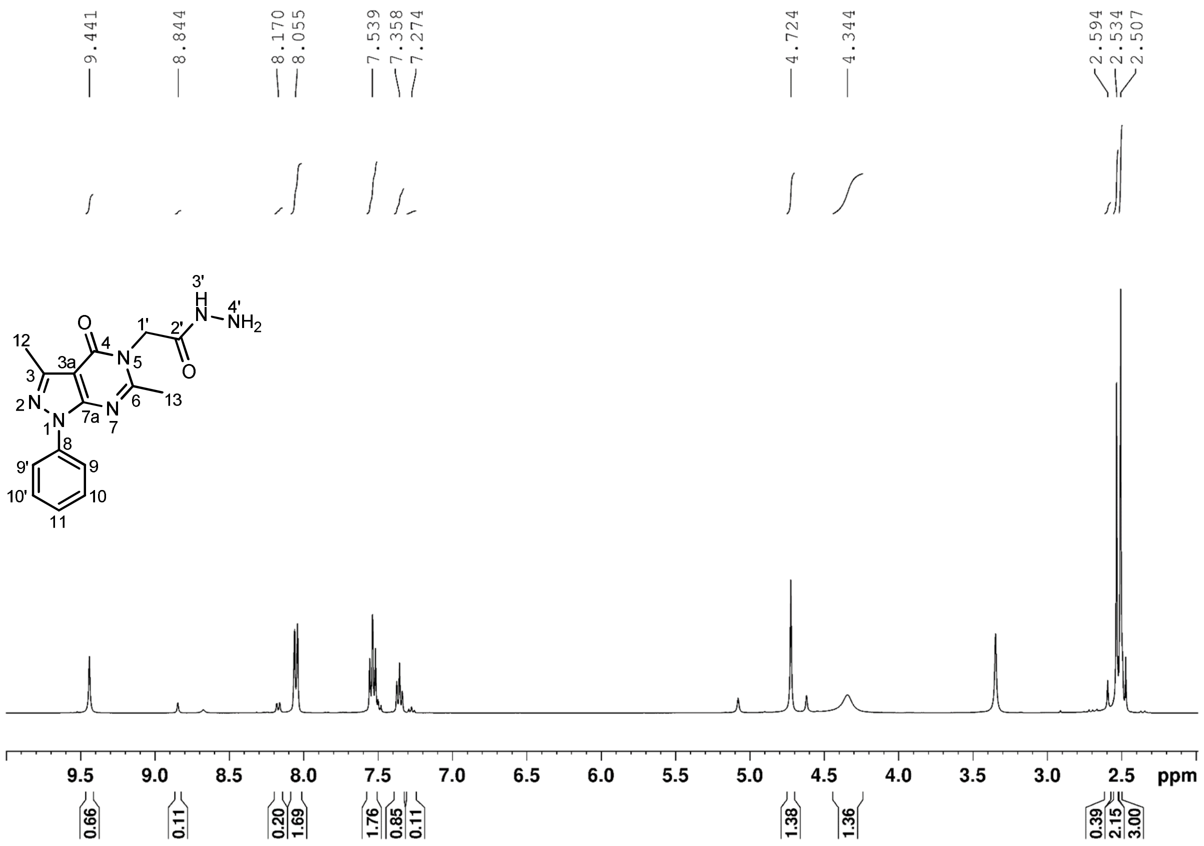

Figure S8. ^{1}H NMR spectrum of compound **4** (DMSO-*d*$_6$, 400MHz).

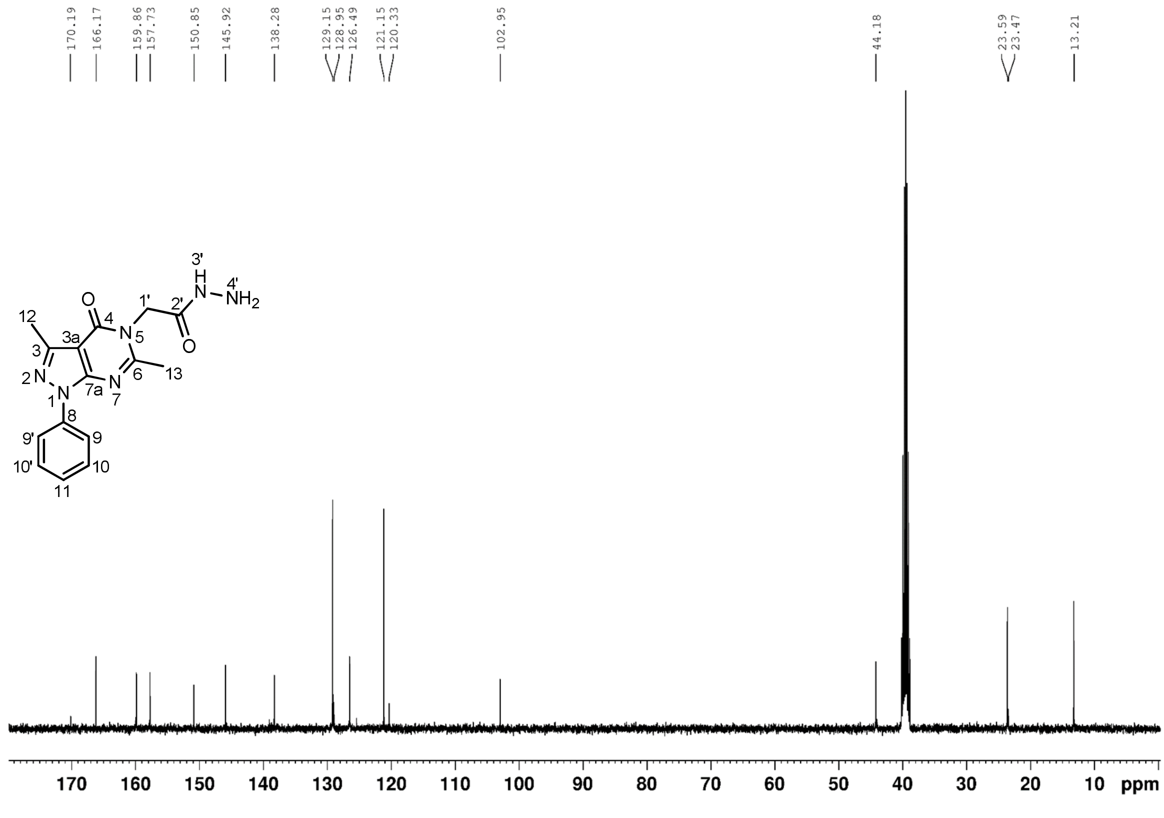

Figure S9. ^{13}C NMR spectrum of compound **4** (DMSO-*d*$_6$, 100MHz).

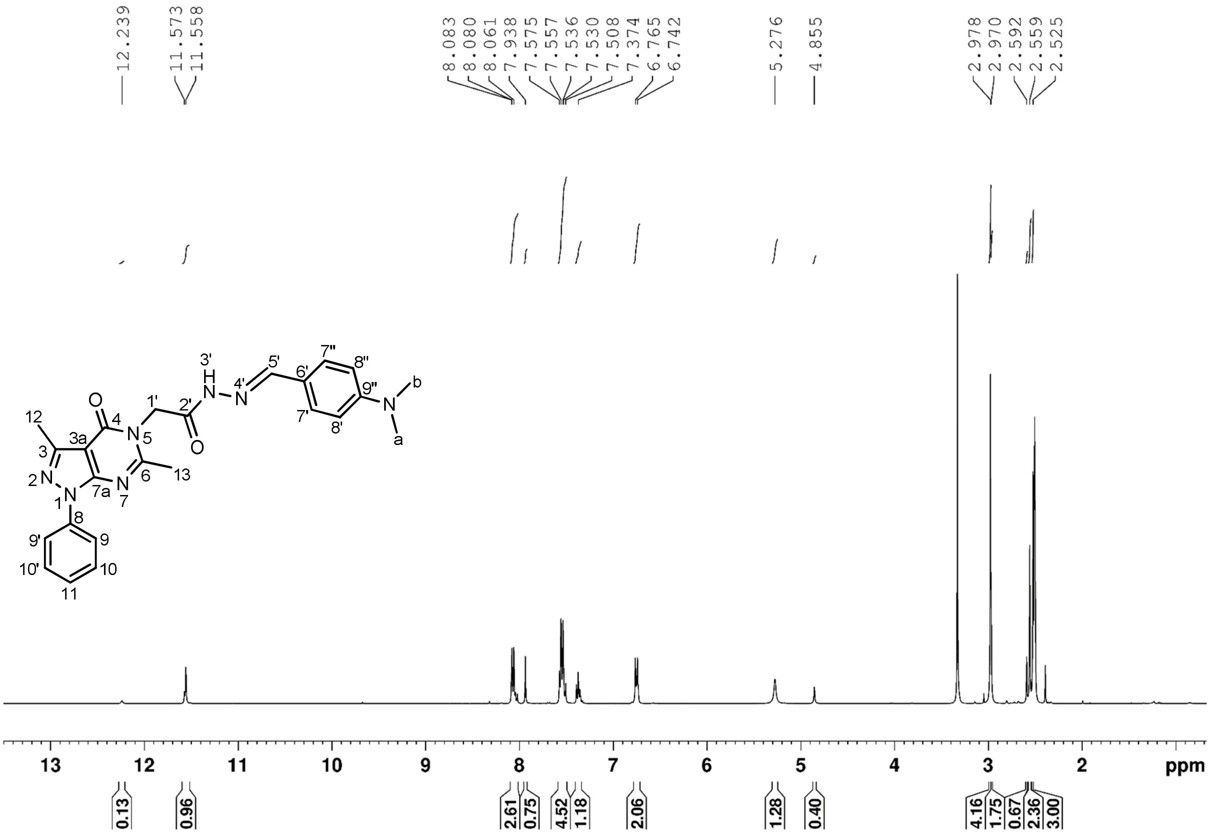

Figure S10. ^{1}H NMR spectrum of compound **5a** (DMSO-d_6, 400MHz).

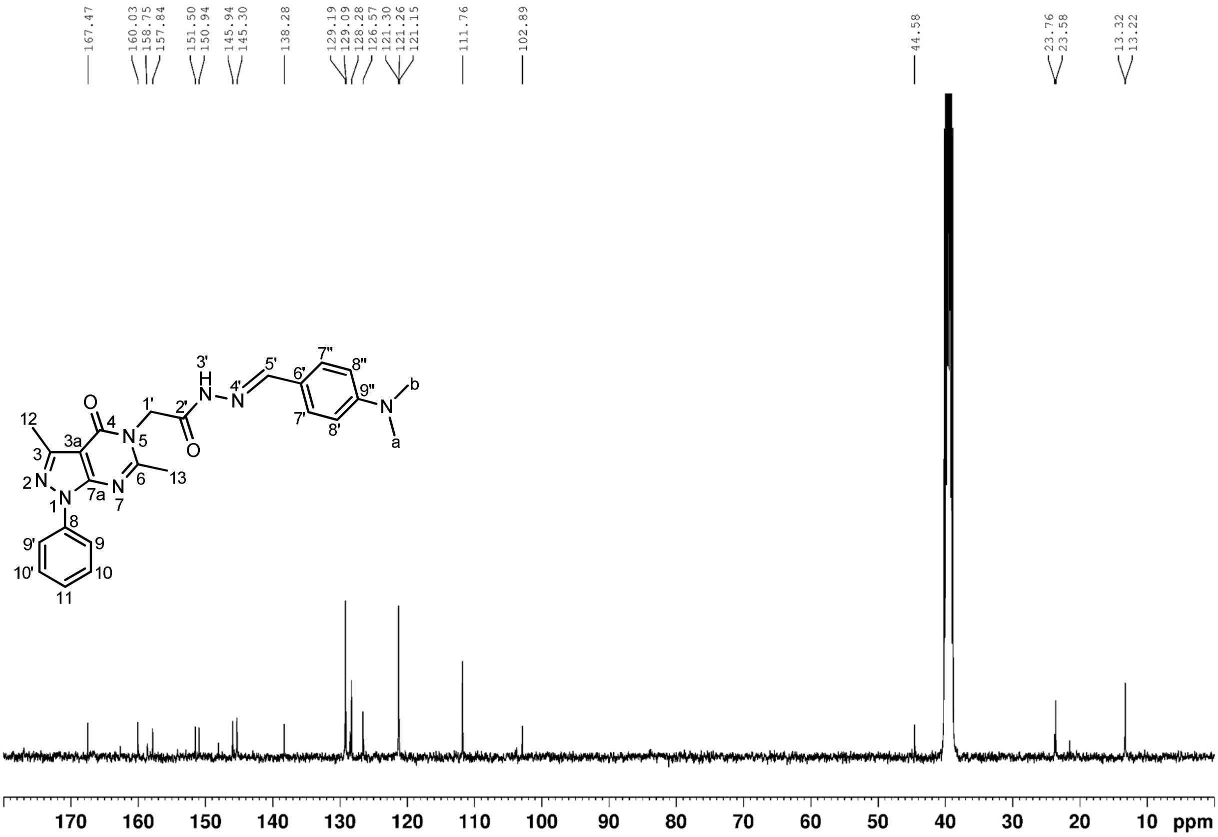

Figure S11. ^{13}C NMR spectrum of compound **5a** (DMSO-d_6, 100MHz).

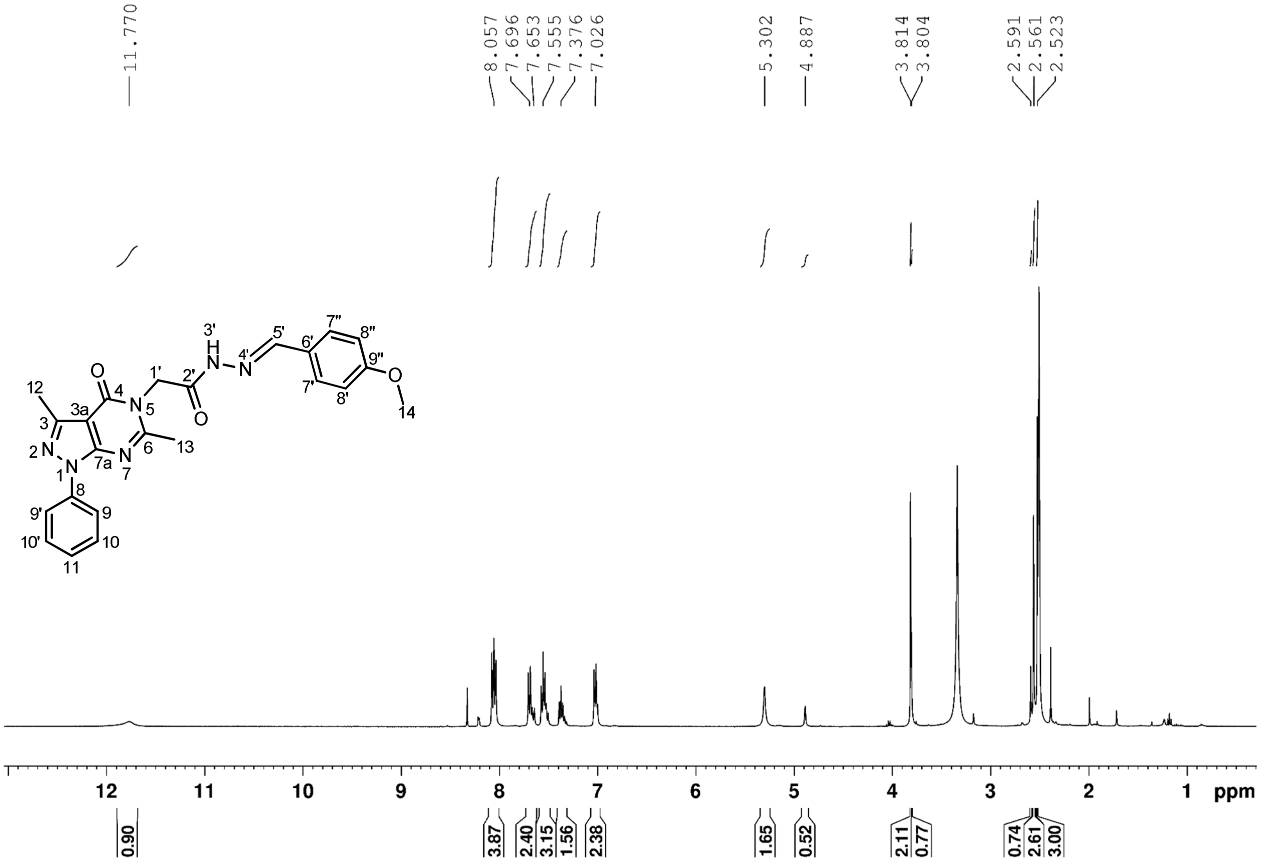

Figure S12. ^{1}H NMR spectrum of compound **5b** (DMSO-d_6, 400MHz).

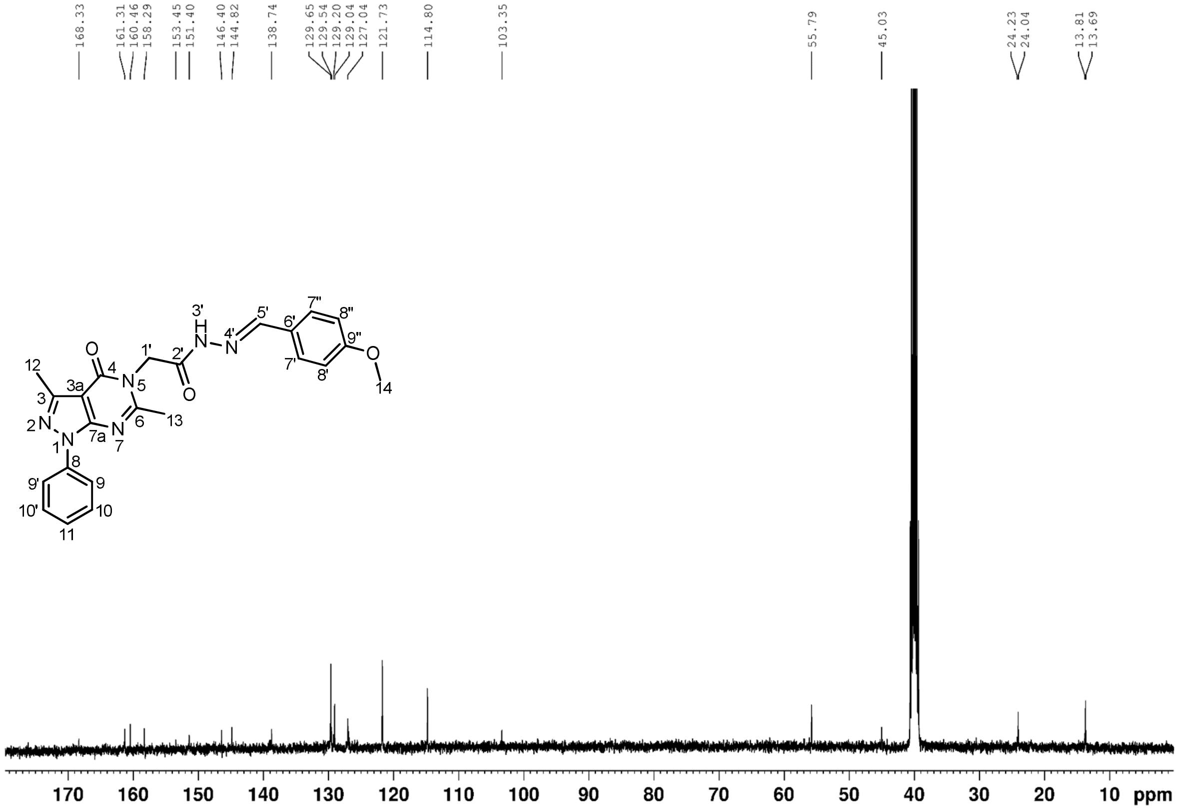

Figure S13. ^{13}C NMR spectrum of compound **5b** (DMSO-d_6, 100MHz).

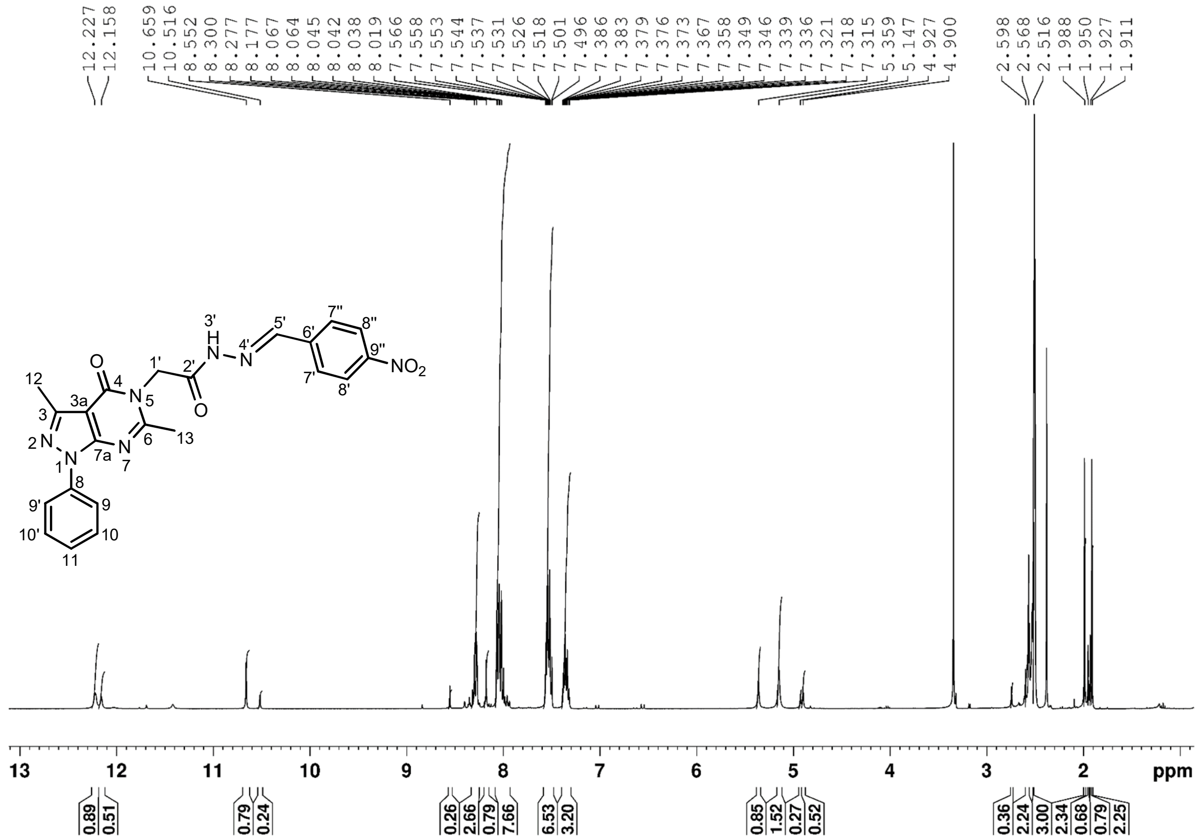

Figure S14. ^1H NMR spectrum of compound **5c** (DMSO-d_6, 400MHz).

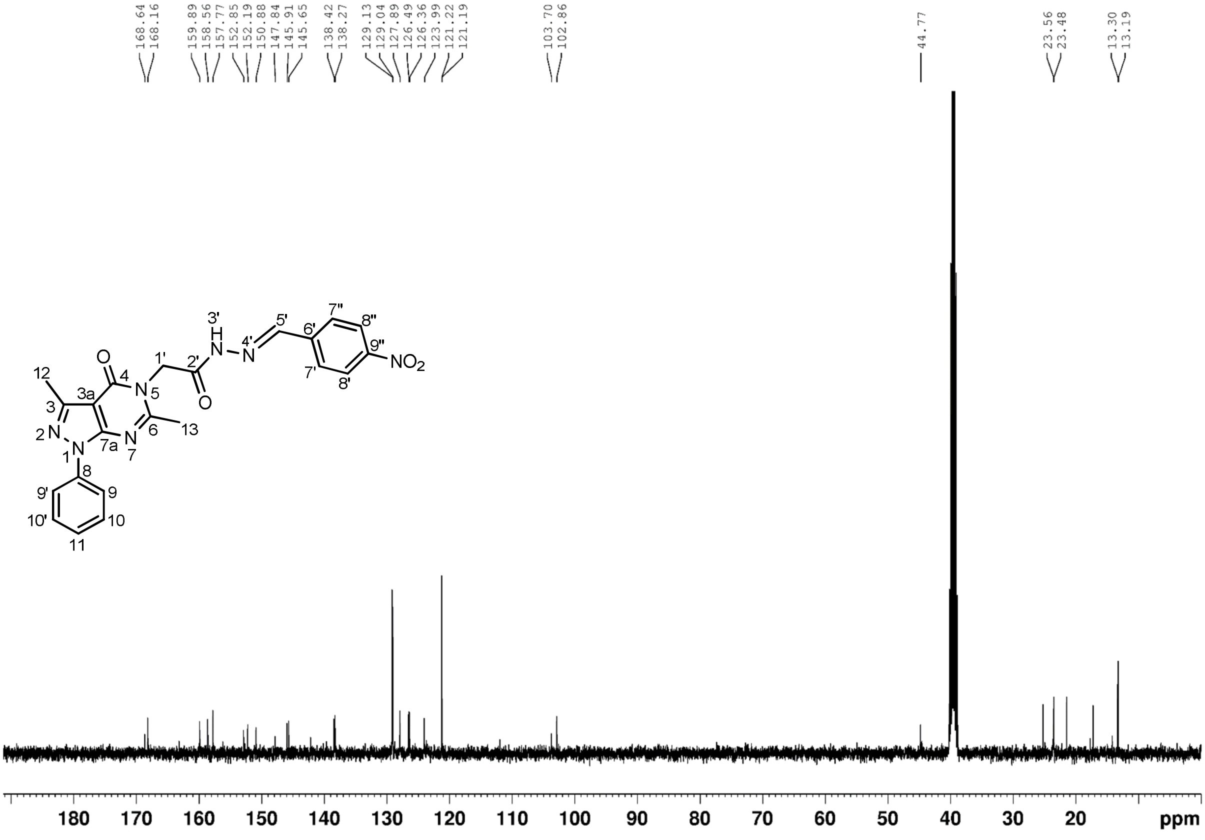

Figure S15. ^{13}C NMR spectrum of compound **5c** (DMSO-d_6, 100MHz).

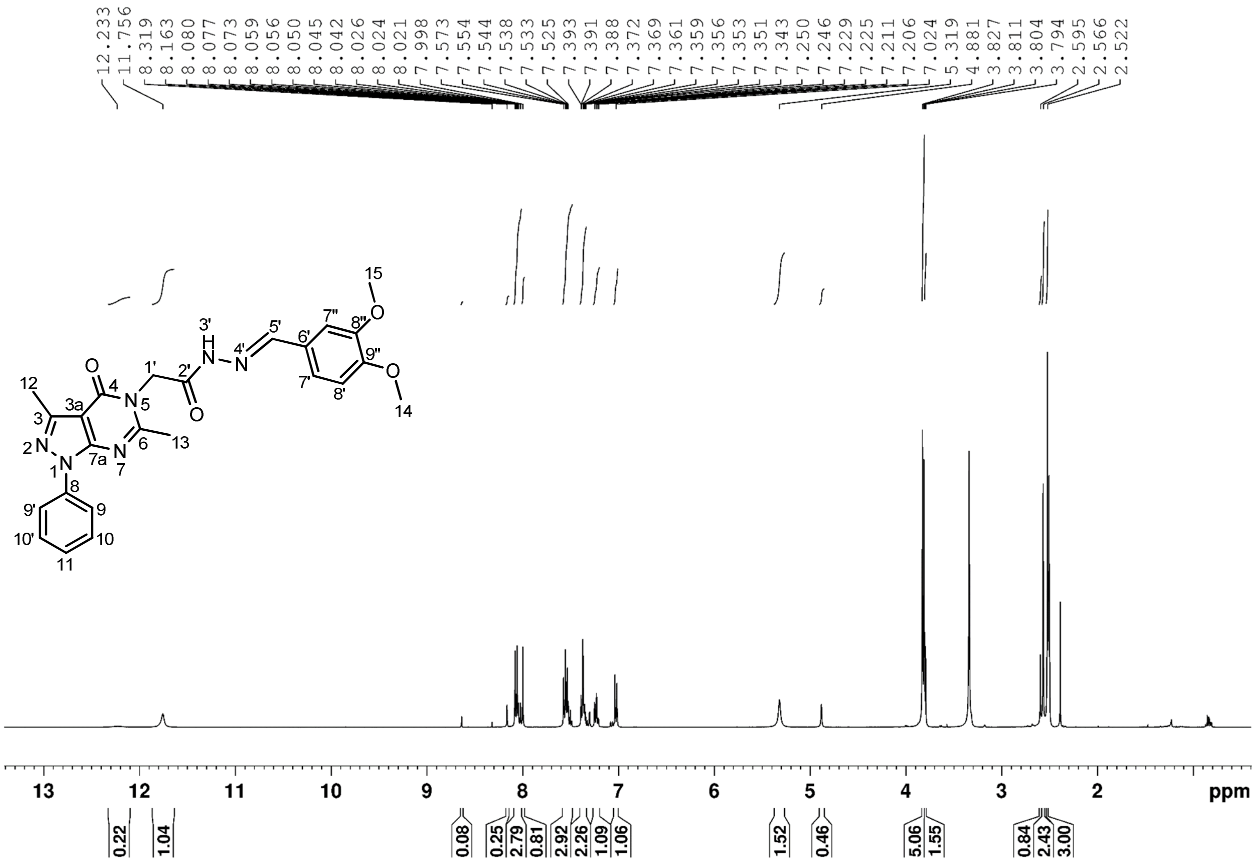

Figure S16. ^{1}H NMR spectrum of compound **5d** (DMSO-d_6, 400MHz).

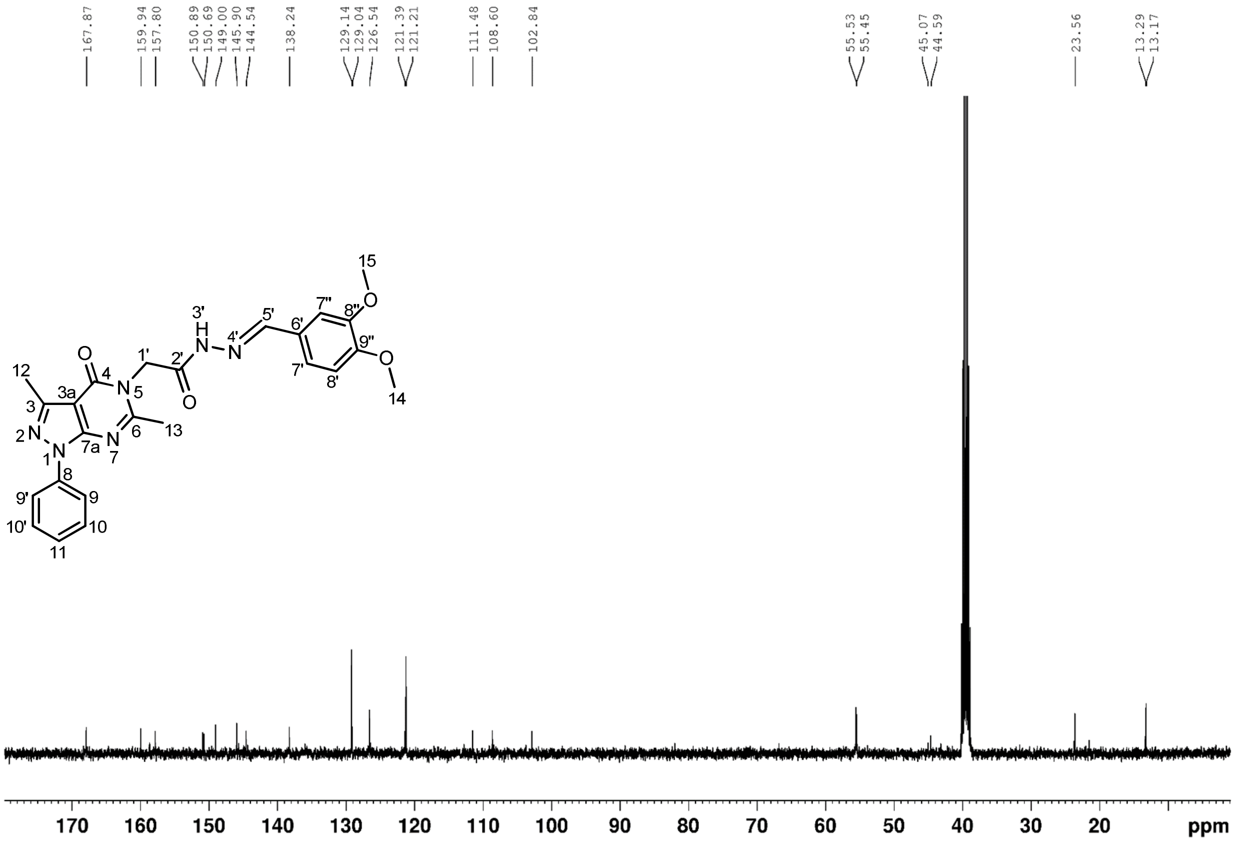

Figure S17. ^{13}C NMR spectrum of compound **5d** (DMSO-d_6, 100MHz).

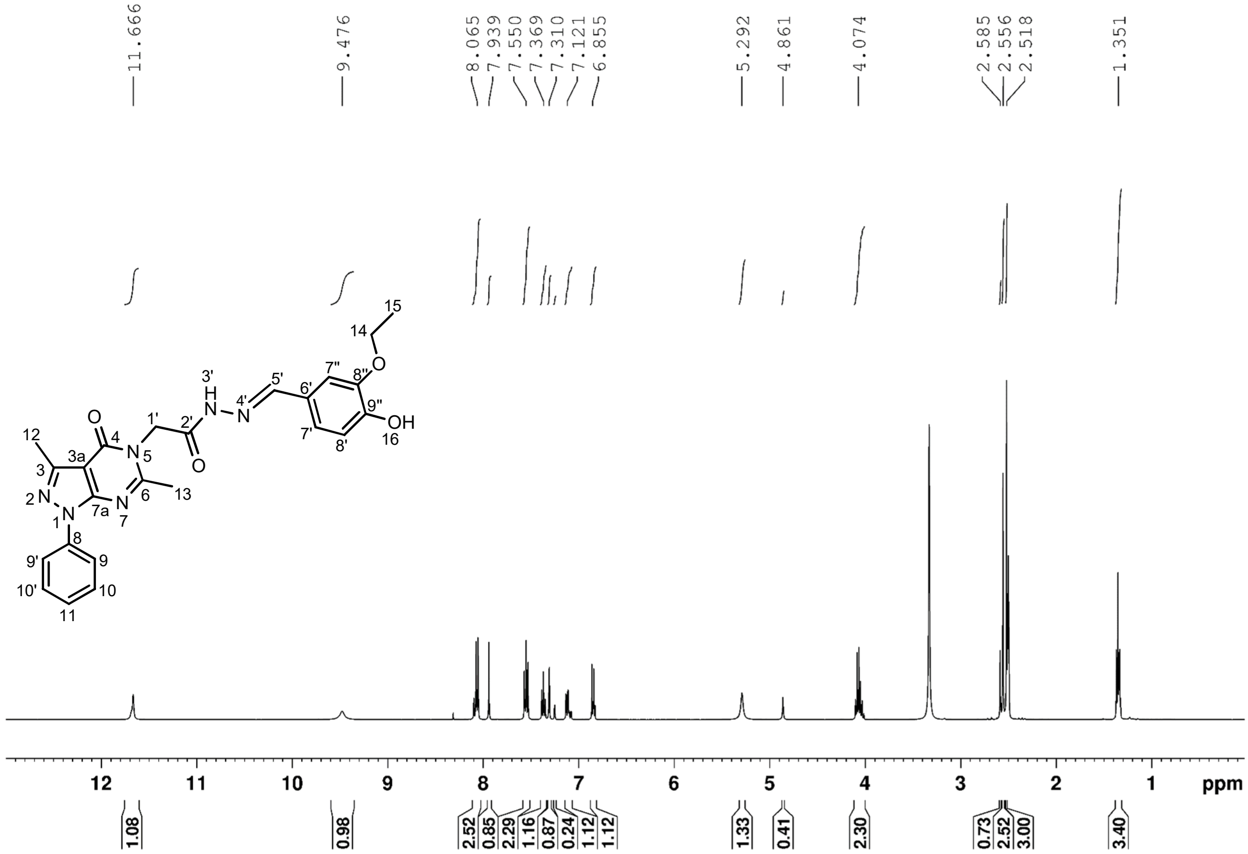

Figure S18. ^{1}H NMR spectrum of compound **5e** (DMSO-d_6, 400MHz).

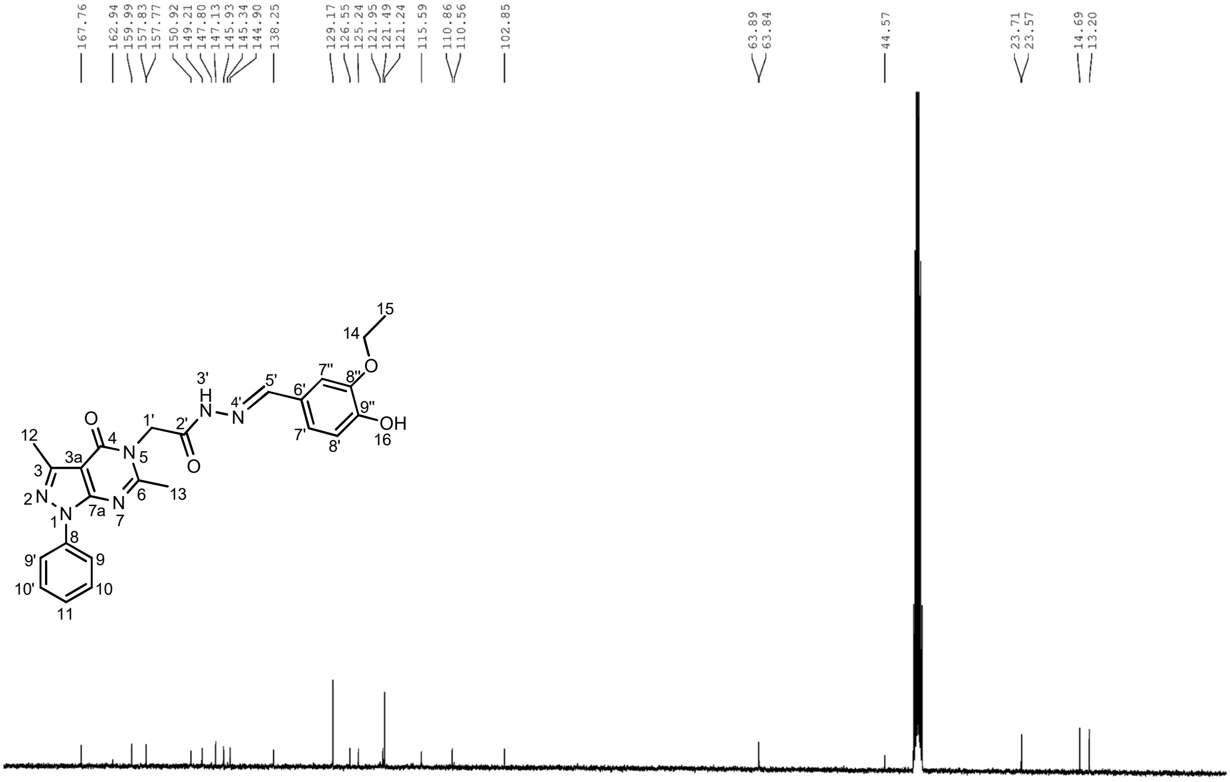

Figure S19. ^{13}C NMR spectrum of compound **5e** (DMSO-d_6, 100MHz).

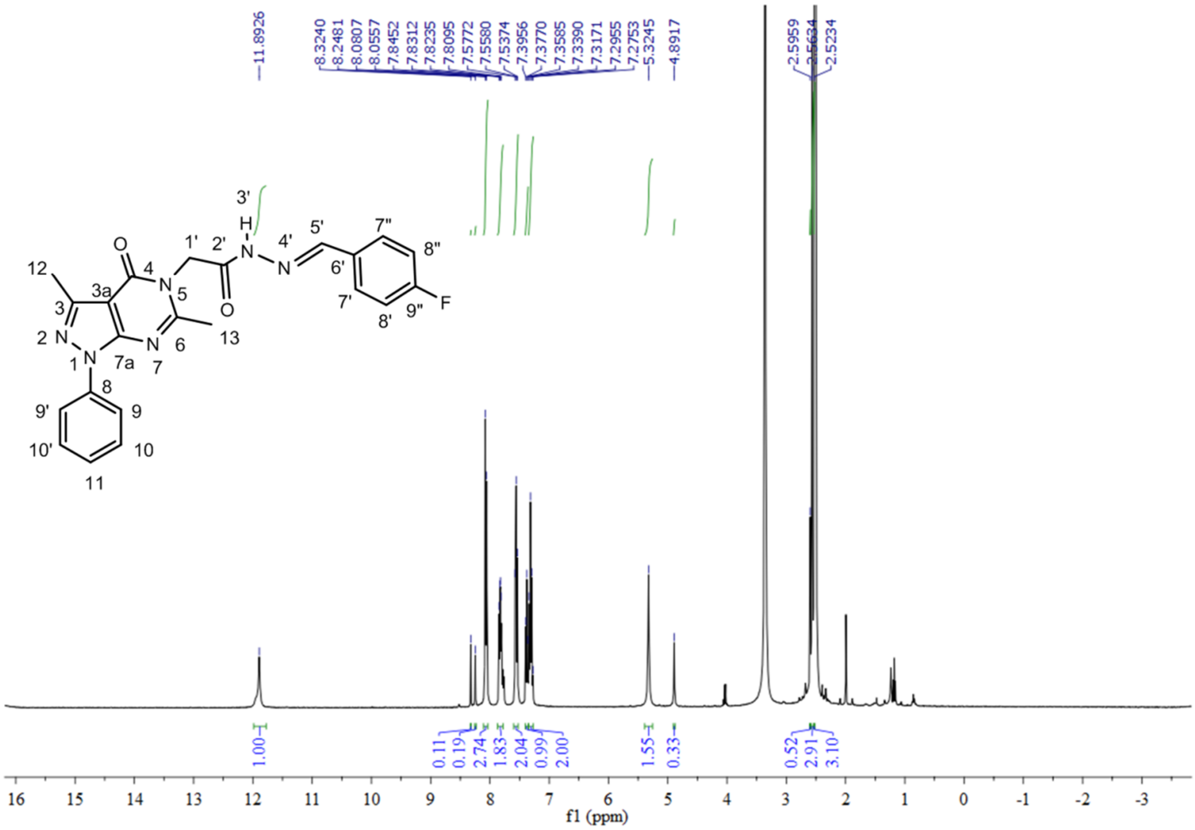

Figure S20. ^{1}H NMR spectrum of compound **5f** (DMSO-*d*$_6$, 400MHz).

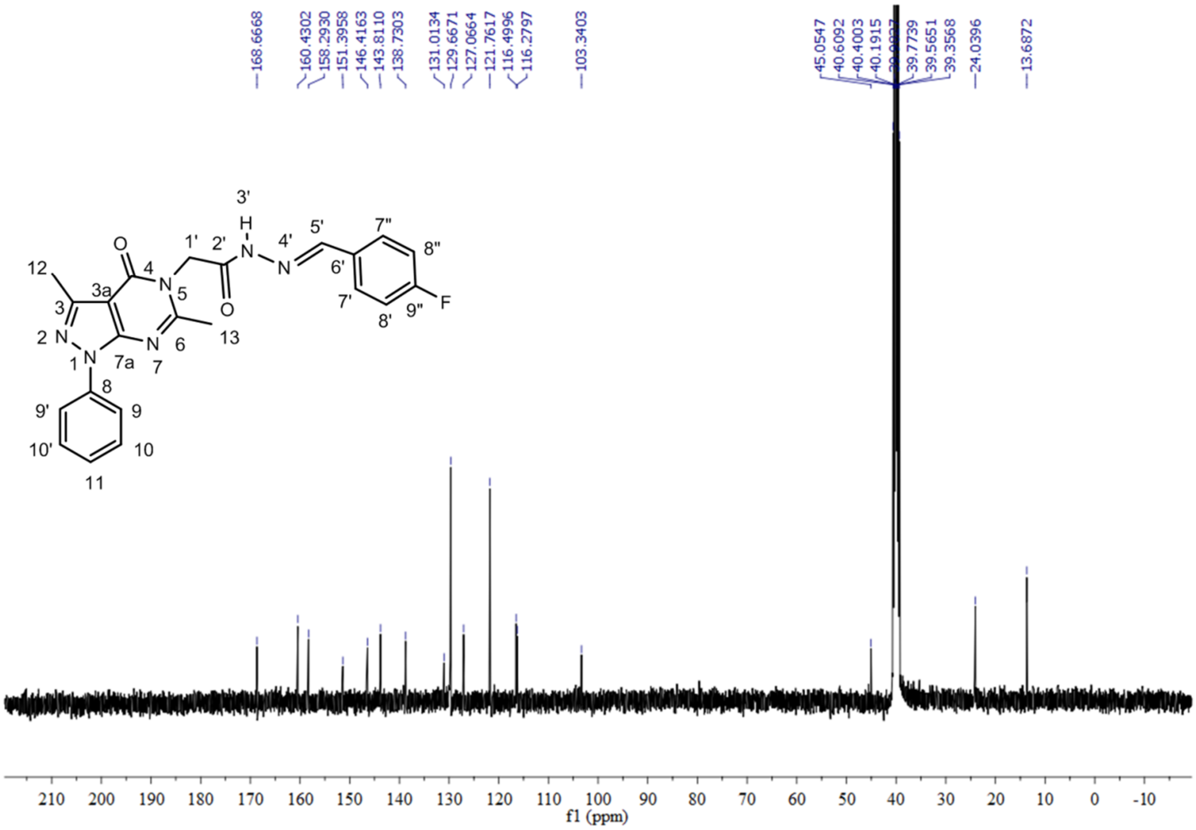

Figure S21. ^{13}C NMR spectrum of compound **5f** (DMSO-*d*$_6$, 100MHz).

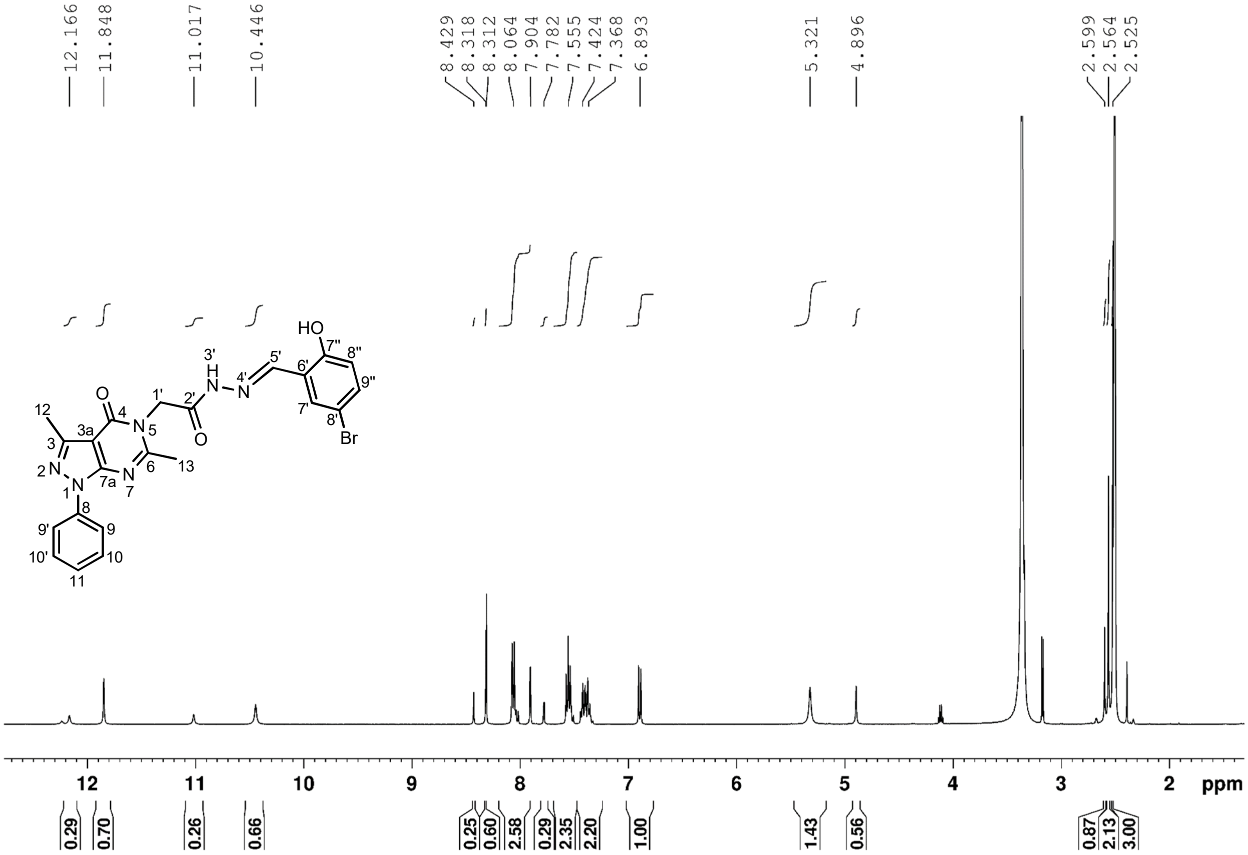

Figure S22. ^{1}H NMR spectrum of compound **5g** (DMSO-*d*$_6$, 400MHz)

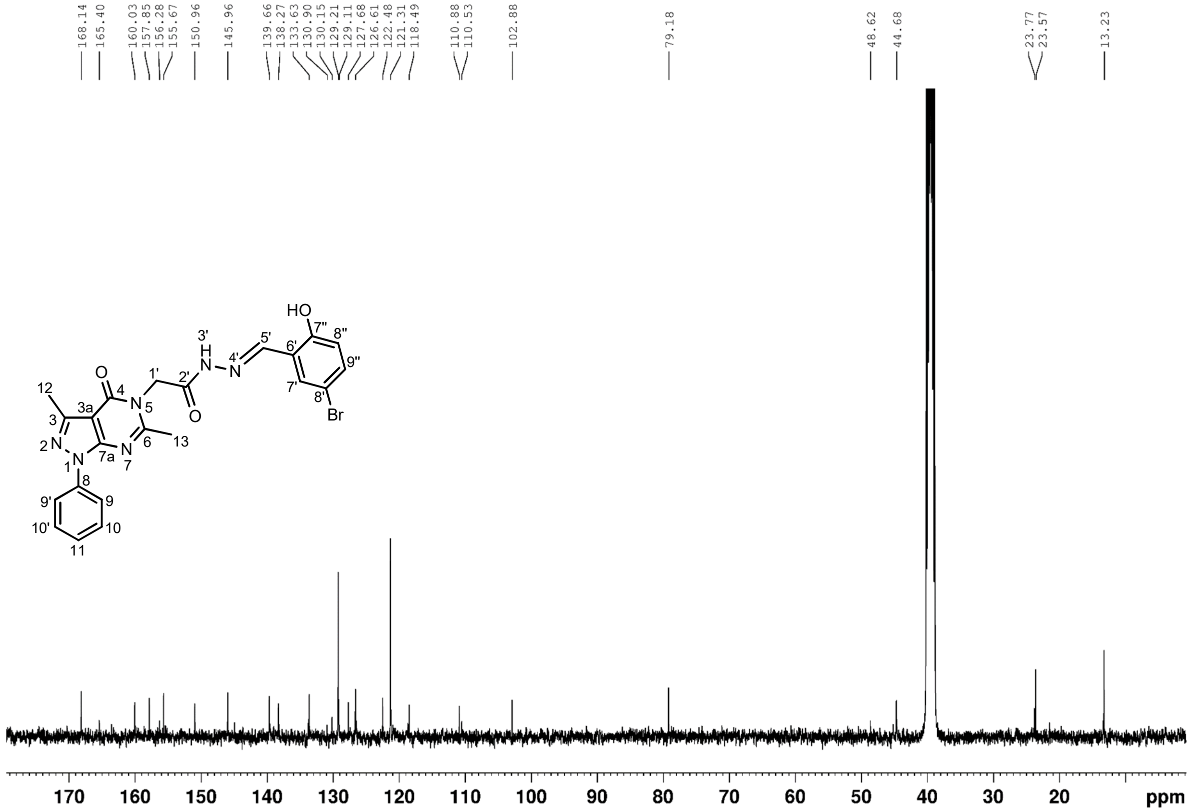

Figure S23. ^{13}C NMR spectrum of compound **5g** (DMSO-*d*$_6$, 100MHz)

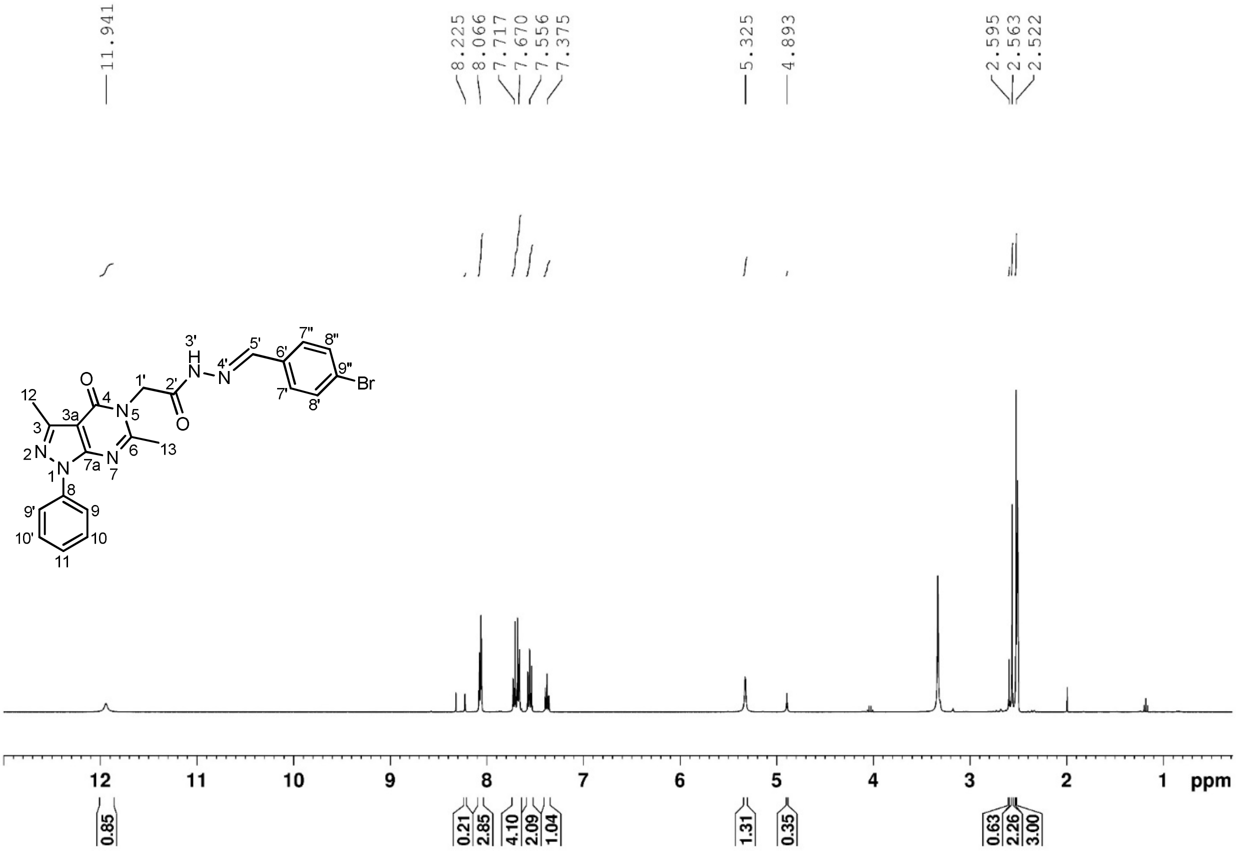

Figure S24. ^{1}H NMR spectrum of compound **5h** (DMSO-*d*$_6$, 400MHz)

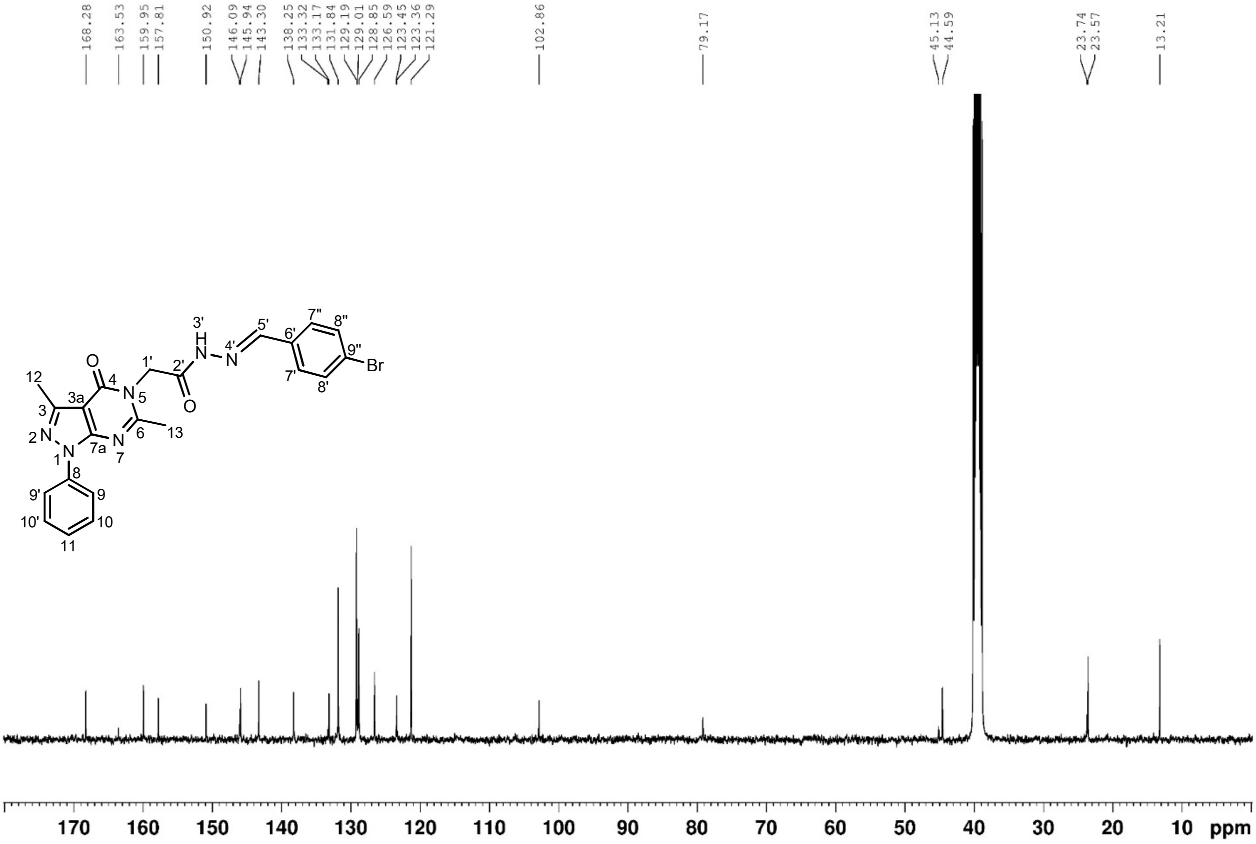

Figure S25. ^{13}C NMR spectrum of compound **5h** (DMSO-*d*$_6$, 100MHz)

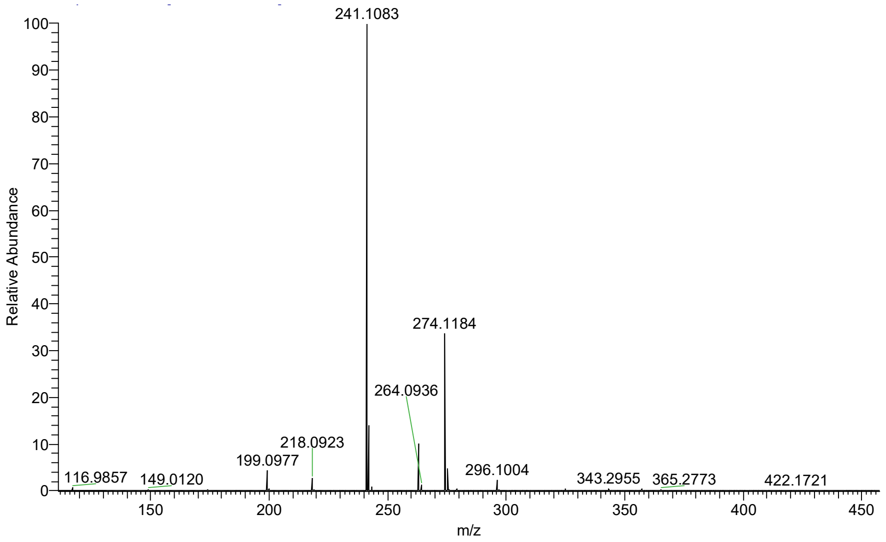

Figure S26. HR-ESI-MS spectrum of compound **2**.

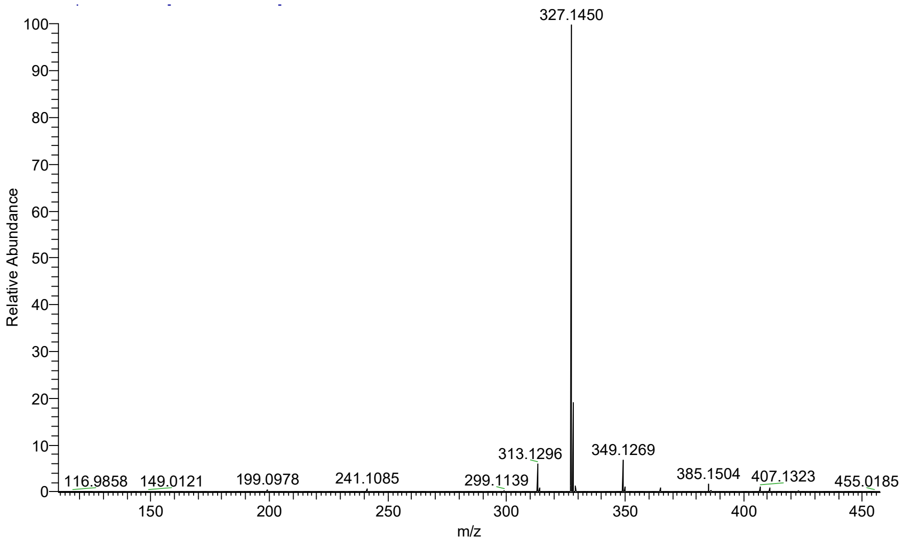

Figure S27. HR-ESI-MS spectrum of compound **3**.

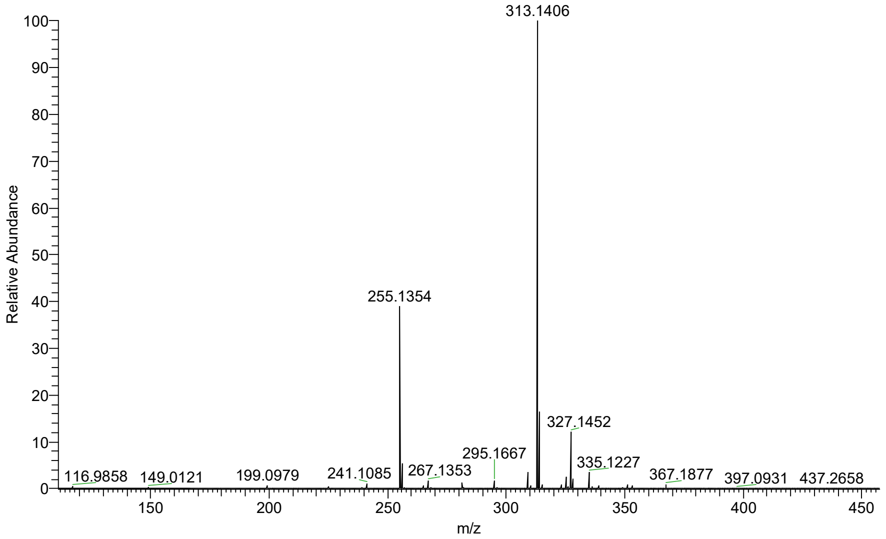

Figure S28. HR-ESI-MS spectrum of compound **4**.

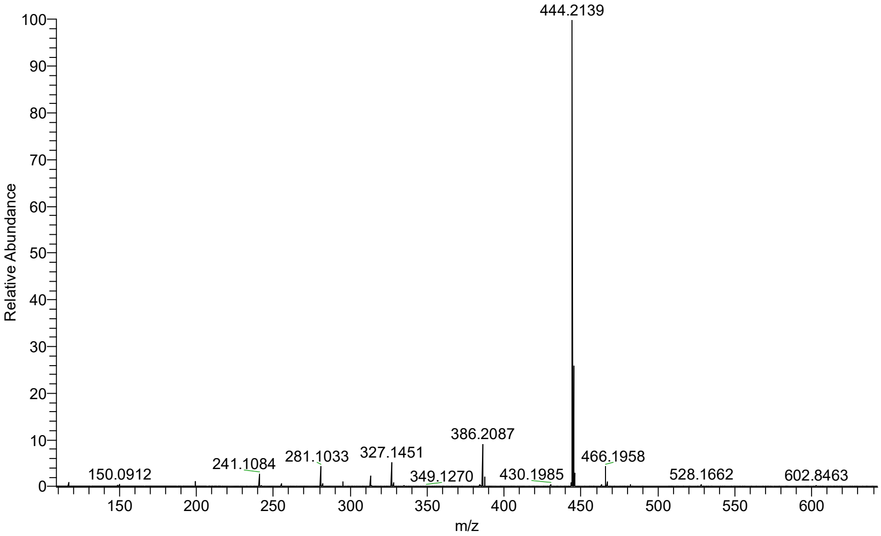

Figure S29. HR-ESI-MS spectrum of compound **5a**.

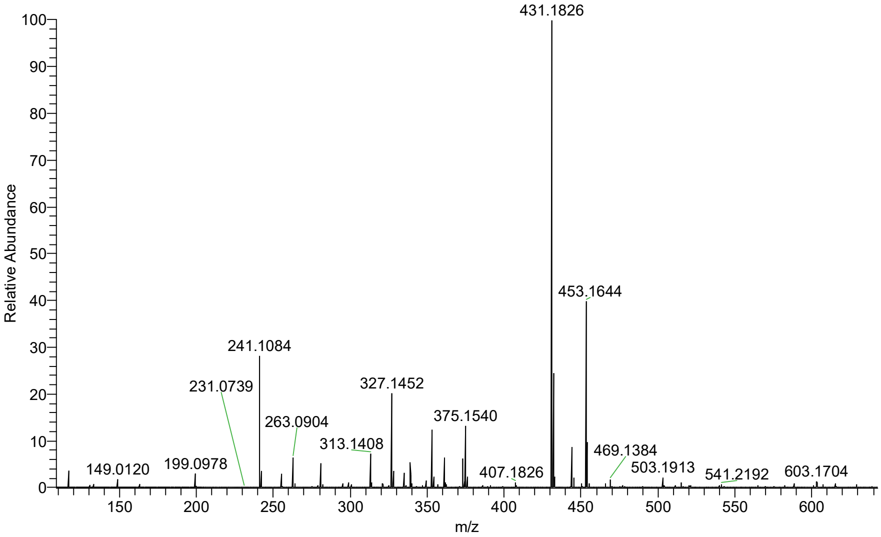

Figure S30. HR-ESI-MS spectrum of compound **5b**.

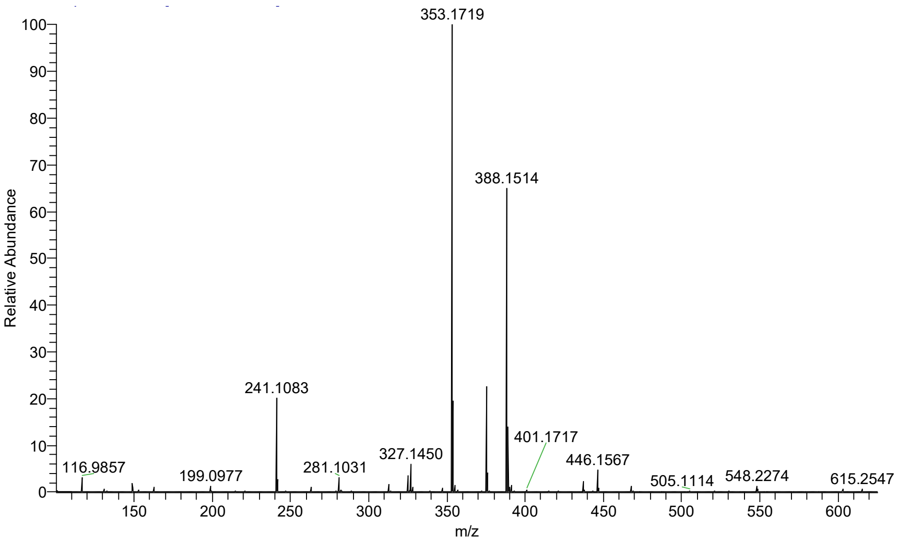

Figure S31. HR-ESI-MS spectrum of compound **5c**.

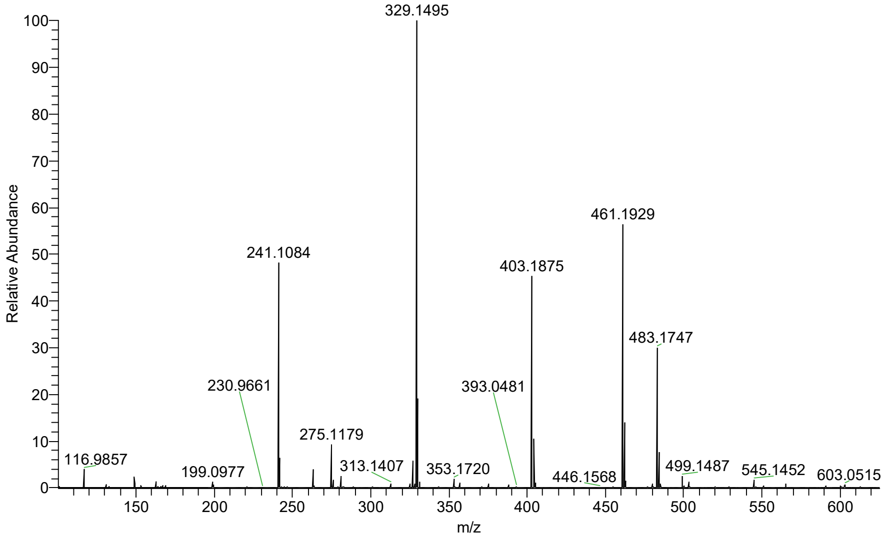

Figure S32. HR-ESI-MS spectrum of compound **5d**.

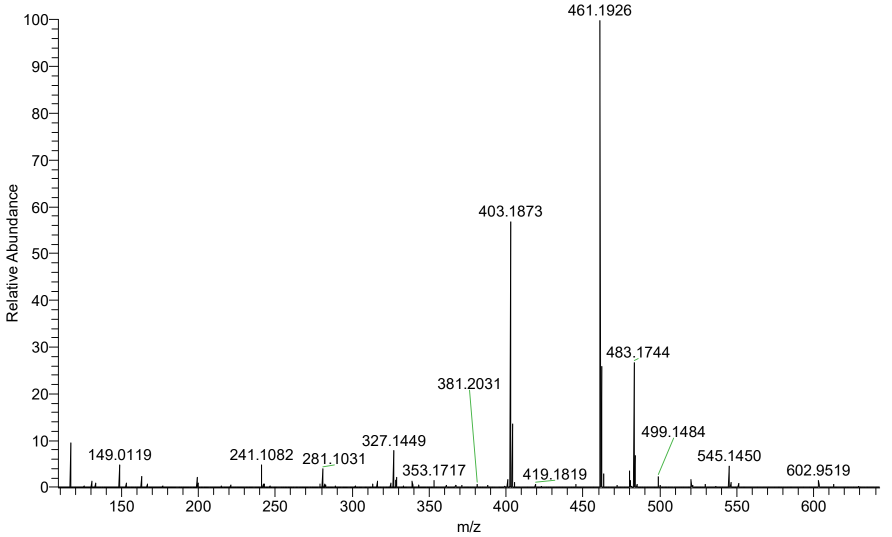

Figure S33. HR-ESI-MS spectrum of compound **5e**.

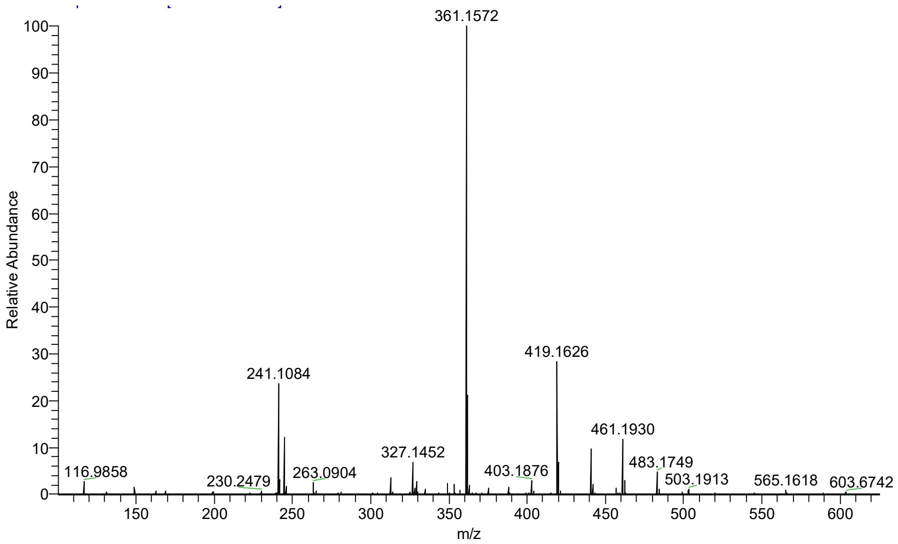

Figure S34. HR-ESI-MS spectrum of compound **5f**.

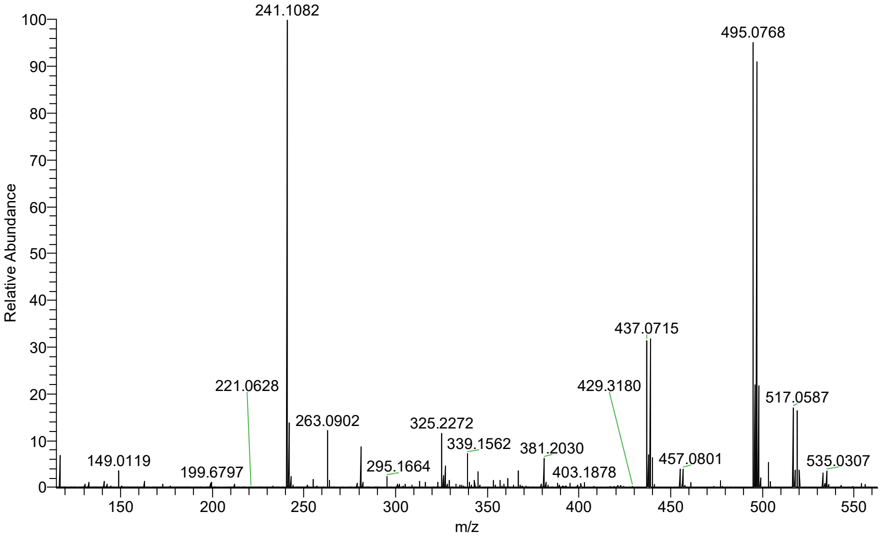

Figure S35. HR-ESI-MS spectrum of compound **5g**.

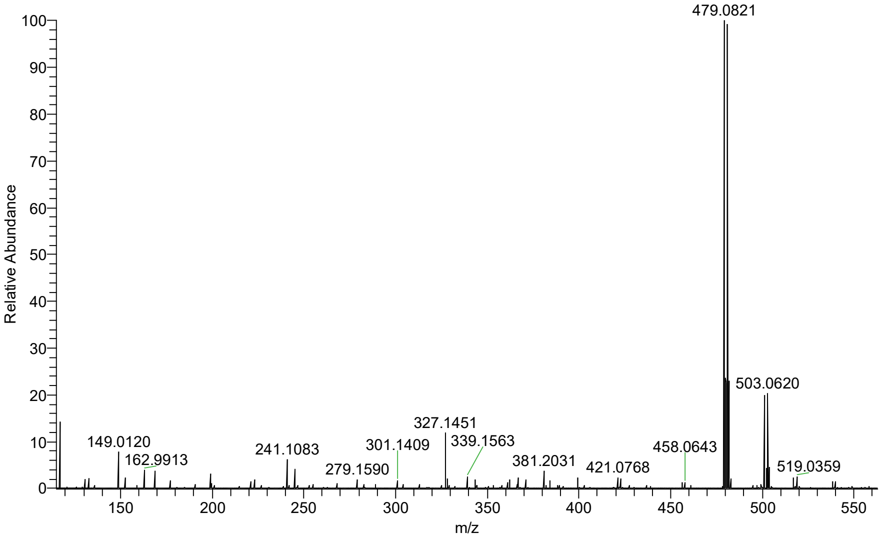

Figure S36. HR-ESI-MS spectrum of compound **5h**.