

SUPPORTING INFORMATION

Potent EGFR/PARP-1 Inhibition by Spirooxindole-Triazole Hybrids for Targeted Liver Cancer Therapy

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X-Ray structure determinations

The crystals of **acetyl-triazole derivative**, **1a**, and **1b** were immersed in cryo-oil, mounted in a loop, and measured at a temperature of 120-121 K. The X-ray diffraction data were collected on a Rigaku Oxford Diffraction Supernova diffractometer using Cu K α radiation (**acetyl-triazole derivative** and **1b**) or Mo K α radiation (**1a**). The *CrysAlisPro*¹ software package was used for cell refinements and data reductions. A multi-scan (**acetyl-triazole derivative** and **1a**) or an analytical (**1b**) absorption correction (*CrysAlisPro*¹) was applied to the intensities before the structure solutions. The structures were solved by the intrinsic phasing (*SHELXT*²) method. Structural refinements were carried out using *SHELXL*³ software with *SHELXLE*⁴ graphical user interface. All hydrogen atoms were positioned geometrically and constrained to ride on their parent atoms, with C-H = 0.95-0.99 Å and $U_{\text{iso}} = 1.2-1.5 \cdot U_{\text{eq}}(\text{parent atom})$. The crystallographic details are summarized in Table S1.

Table S1. Crystal Data of **acetyl-triazole derivative**, **1a**, and **1b**.

	acetyl-triazole derivative	1a	1b
CCDC	2360616	2360617	2360618
empirical formula	C ₁₁ H ₈ Cl ₃ N ₃ O	C ₂₀ H ₁₂ Cl ₃ N ₃ O ₂	C ₂₀ H ₁₂ Cl ₃ N ₃ OS
fw	304.55	432.68	448.74
temp (K)	121(2)	120(2)	120(2) K
λ (Å)	1.54184	0.71073	1.54184 Å
cryst syst	Monoclinic	Monoclinic	Monoclinic
space group	<i>P2₁/n</i>	<i>P2₁</i>	<i>I2/a</i>
<i>a</i> (Å)	10.62874(18)	7.66680(10)	25.8395(3)
<i>b</i> (Å)	10.43514(18)	13.8977(2)	7.12869(6)
<i>c</i> (Å)	11.62031(19)	9.5441(2)	23.3863(2)
α (deg)			
β (deg)	93.7149(15)	111.742(2)	114.7797(13)
γ (deg)			
<i>V</i> (Å ³)	1286.13(4)	944.59(3)	3911.17(8)
Z	4	2	8

ρ_{calc} (Mg/m ³)	1.573	1.521	1.524
μ (Mo K α) (mm ⁻¹)	6.387	0.507	5.383
No. reflns.	16383	19035	63498
Unique reflns.	2740	9361	4221
Completeness $\theta=67.684^\circ$	to 100 %		100 %
Completeness $\theta=25.242^\circ$	to	100 %	
Absolute parameter	structure	-0.019(18)	
GOOF (F ²)	1.072	1.033	1.098
R _{int}	0.0343	0.0270	0.0333
R1 ^a ($I \geq 2\sigma$)	0.0309	0.0373	0.0289
wR2 ^b ($I \geq 2\sigma$)	0.0839	0.0772	0.0790

$$^a R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|. \quad ^b wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/ \Sigma[w(F_o^2)^2]\}^{1/2}$$

References

1. Rigaku Oxford Diffraction, *CrysAlisPro 1.171.43.100a*, 2023, Rigaku Oxford Diffraction inc., Yarnton, Oxfordshire, England.
2. Sheldrick, G. M. *Acta Cryst.* **2015**, *A71*, 3-8.
3. Sheldrick, G. M. *Acta Cryst.* **2015**, *C71*, 3-8.
4. Hübschle, C. B.; Sheldrick, G. M.; Dittrich, B. *J. Appl. Cryst.* **2011**, *44*, 1281-1284.

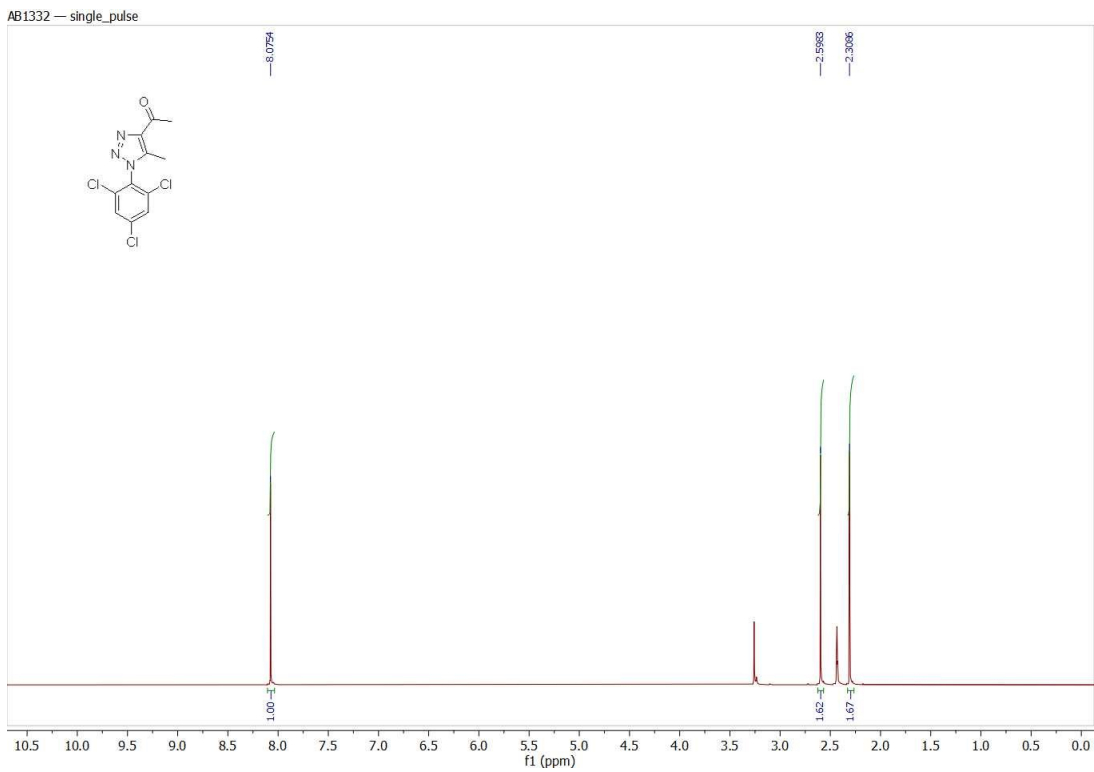


Figure S1: ^1H NMR (DMSO- d_6) for acetyl-triazole derivative

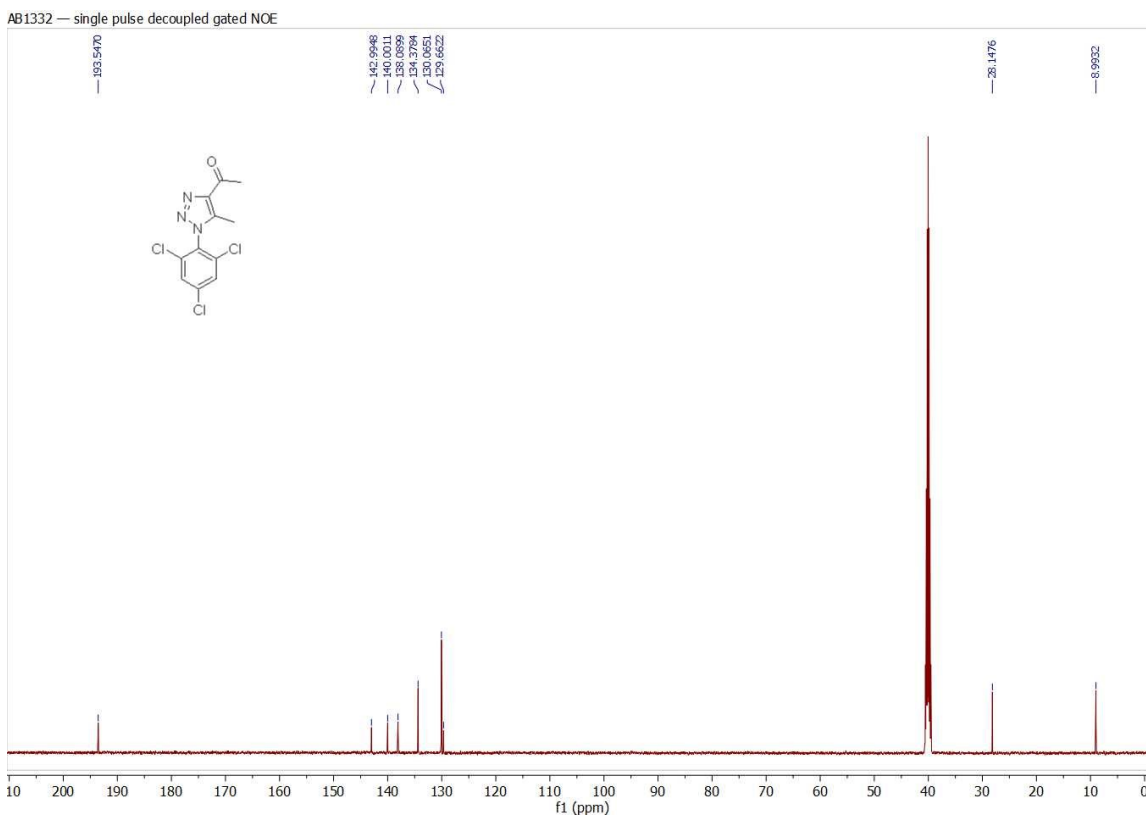


Figure S2: ^{13}C NMR (DMSO- d_6) for acetyl-triazole derivative

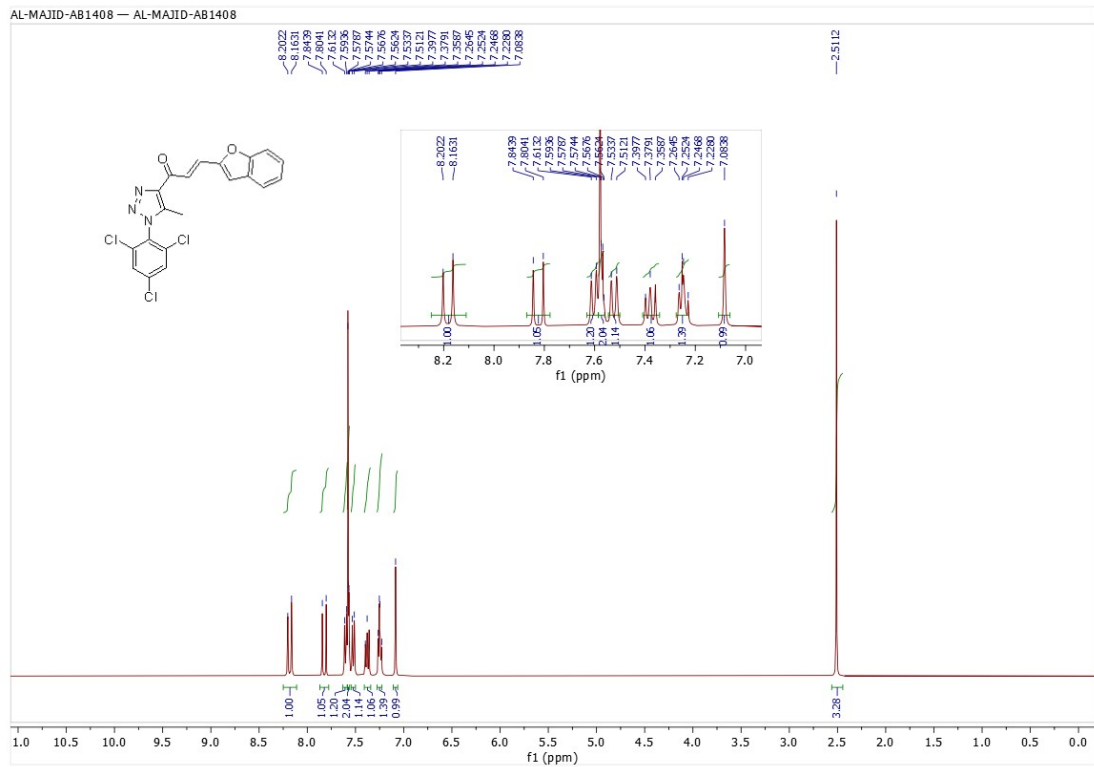


Figure S3: ¹H NMR (CDCl₃) for **1a**

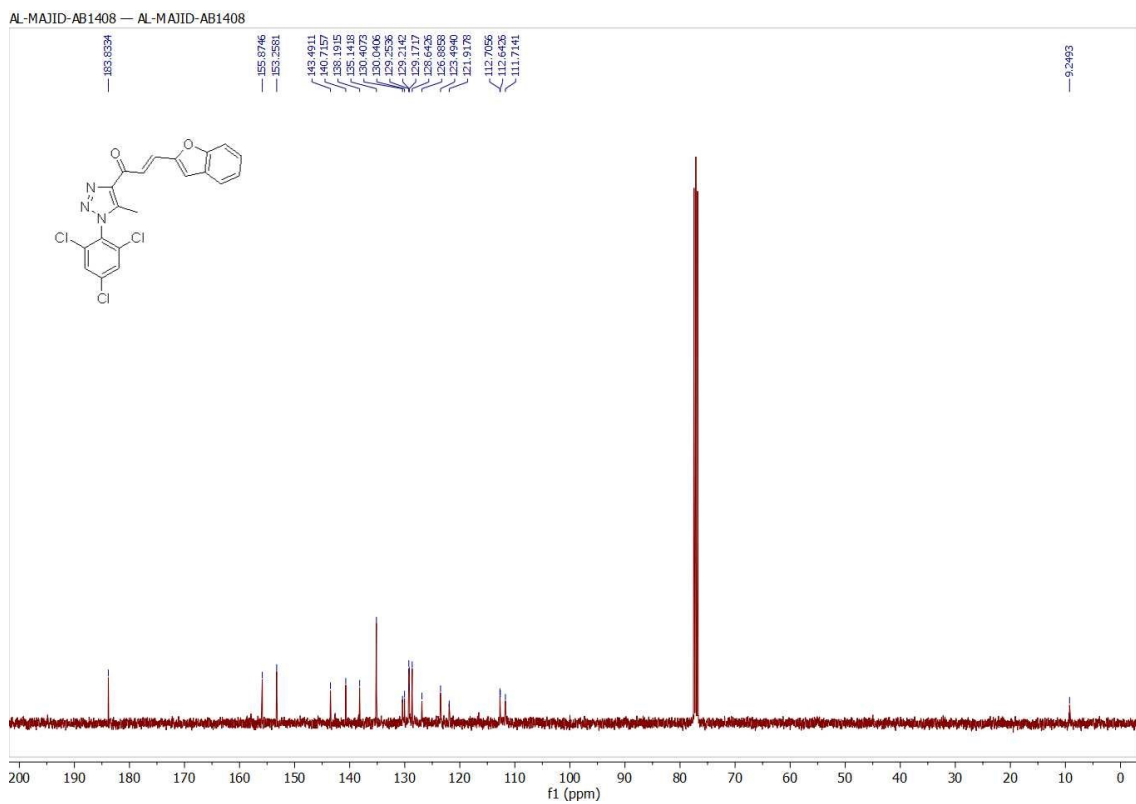


Figure S4: ¹³C NMR (CDCl₃) for **1a**

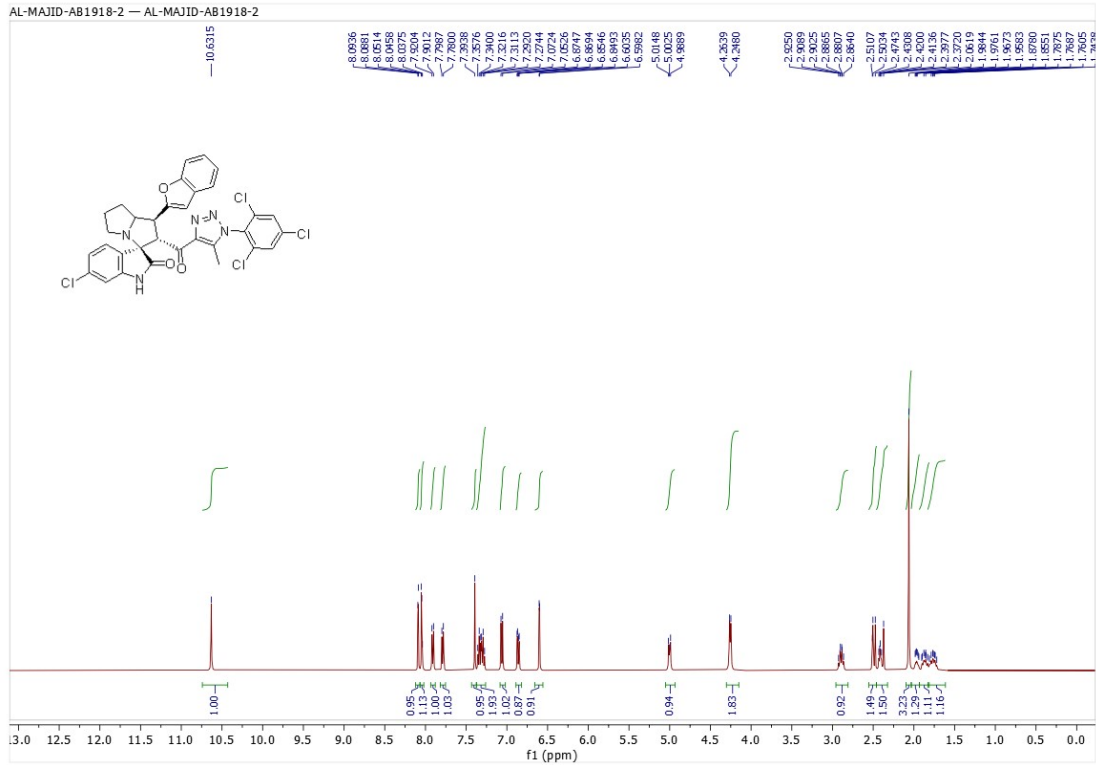


Figure S7: ^1H NMR ($\text{DMSO}-d_6$) for 4a

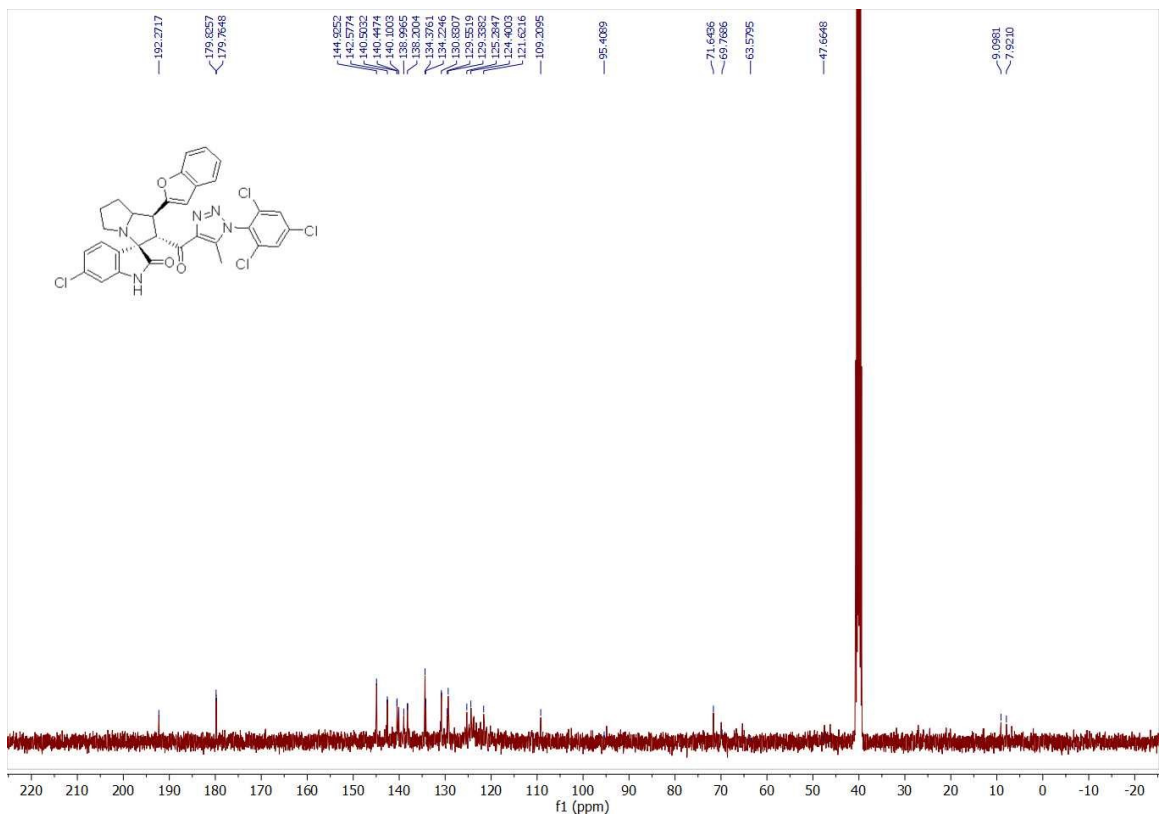


Figure S8: ^{13}C NMR ($\text{DMSO}-d_6$) for 4a

AL-MAJID-AB1419 — AL-MAJID-AB1419

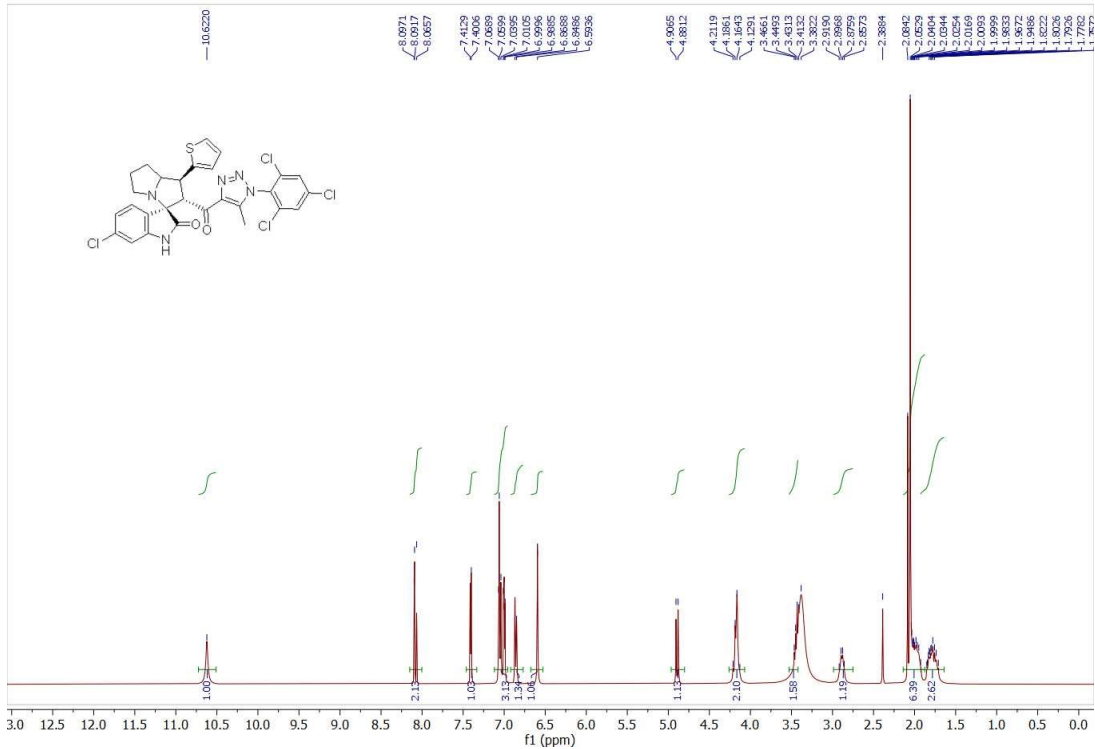


Figure S9: ¹H NMR (DMSO-*d*₆) for 4c

AL-MAJID-AB1419 — AL-MAJID-AB1419

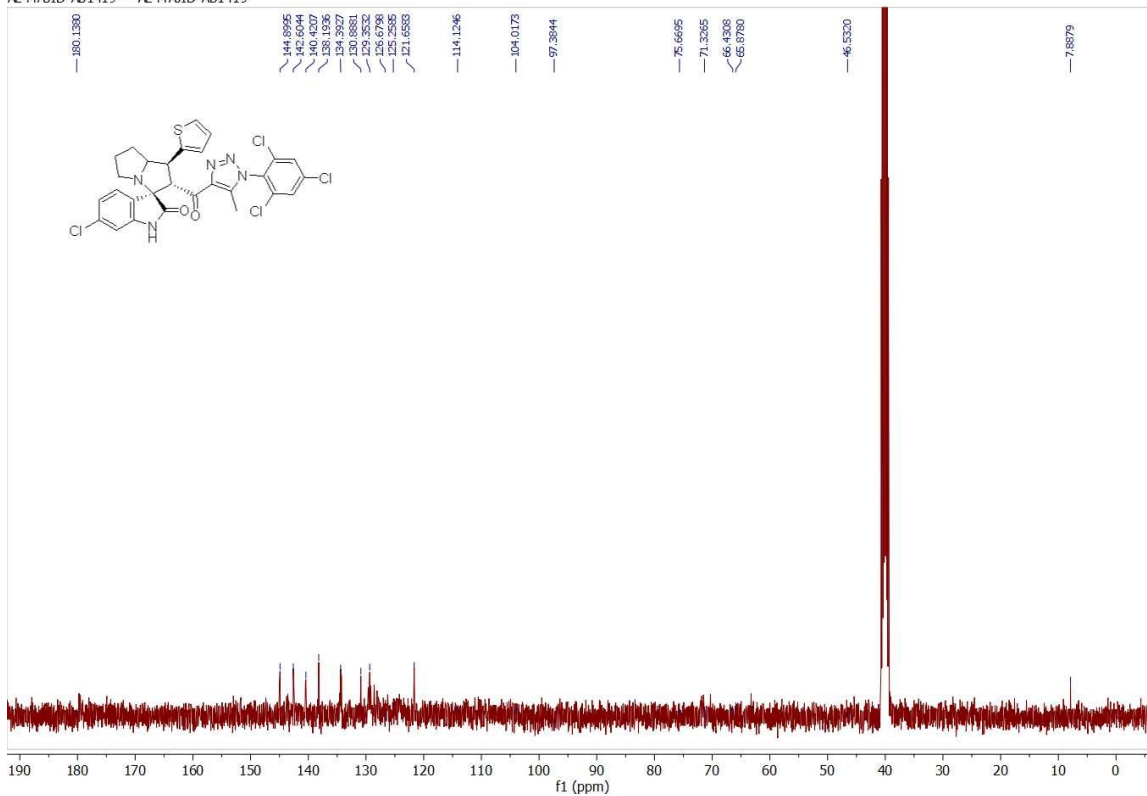


Figure S10: ¹³C NMR (DMSO-*d*₆) for 4c

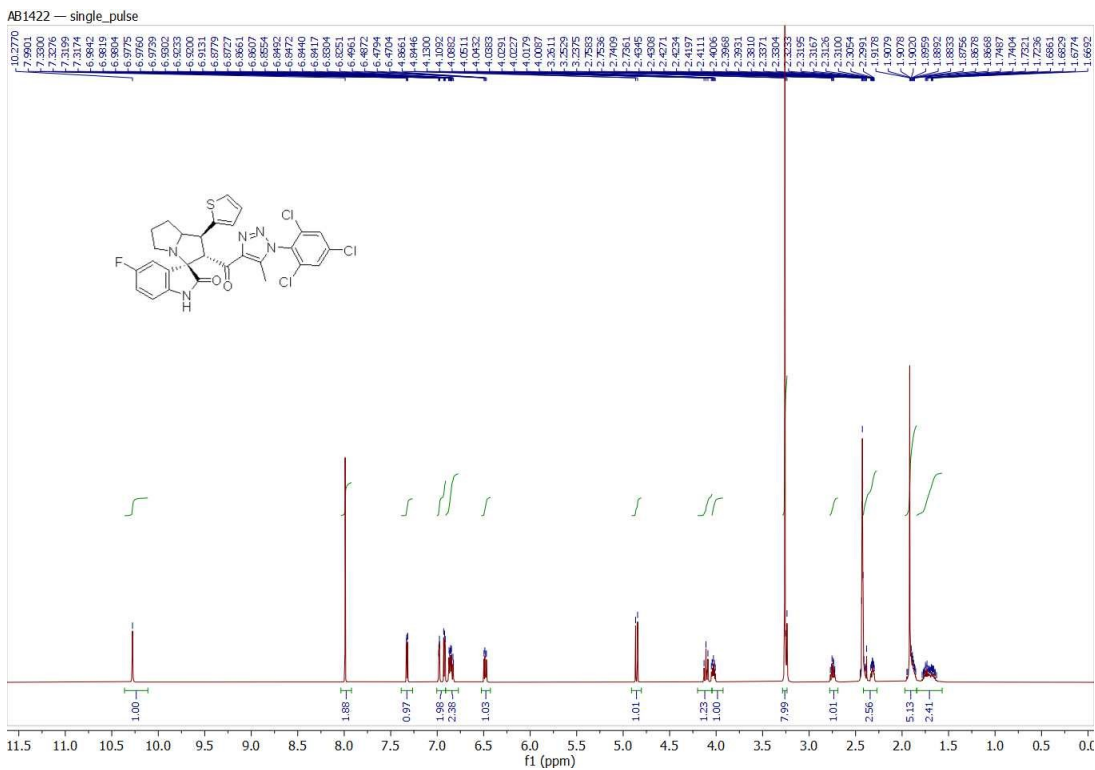


Figure S11: ^1H NMR (DMSO- d_6) for 4d

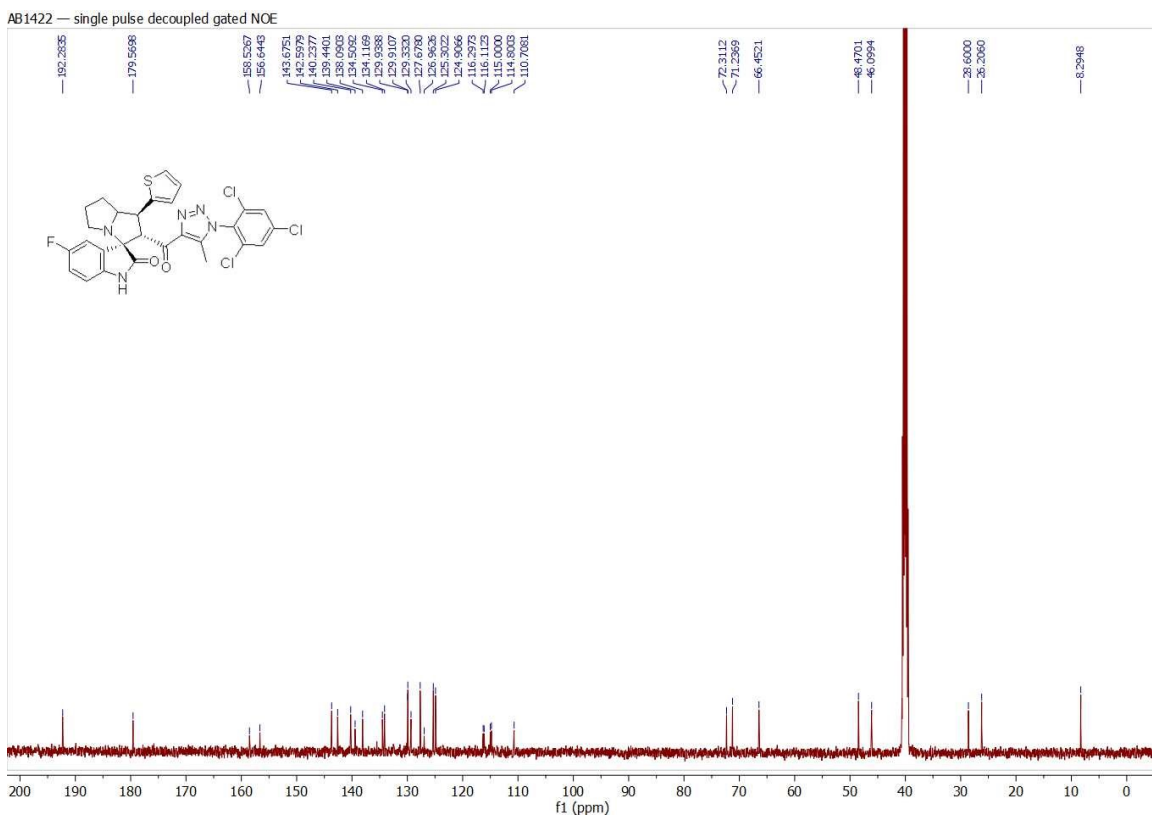


Figure S12: ^{13}C NMR (DMSO- d_6) for 4d

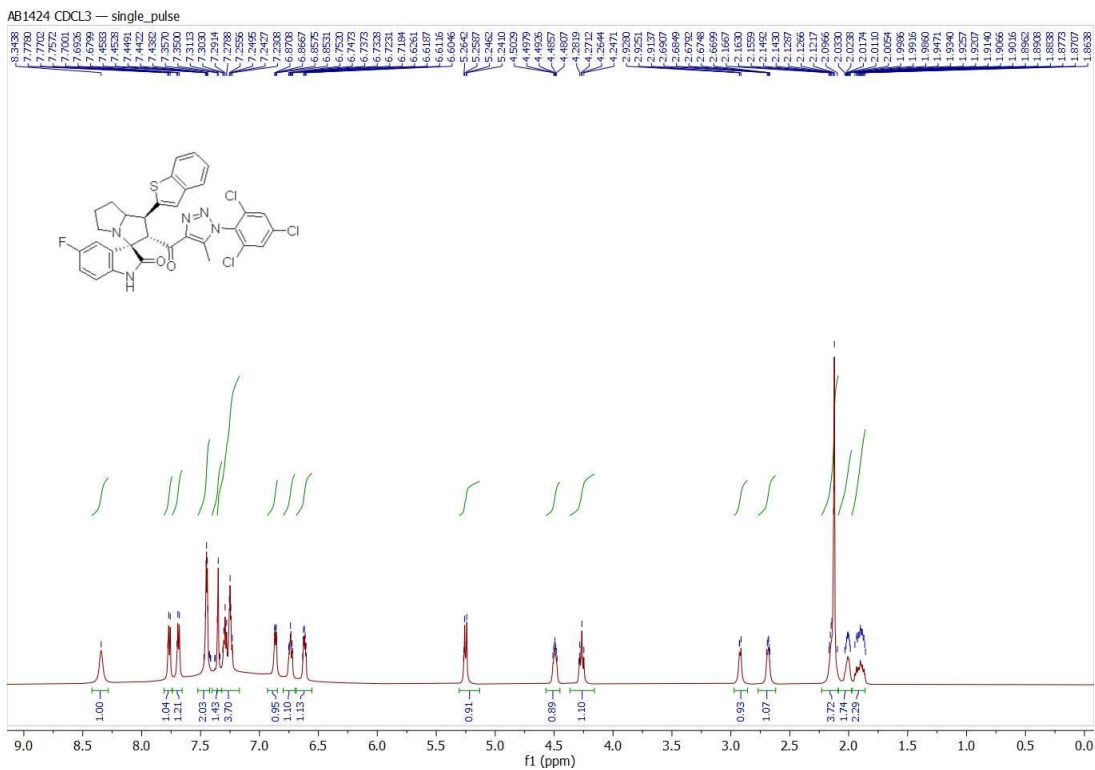


Figure S15: ¹H NMR (DMSO-*d*₆) for 4f

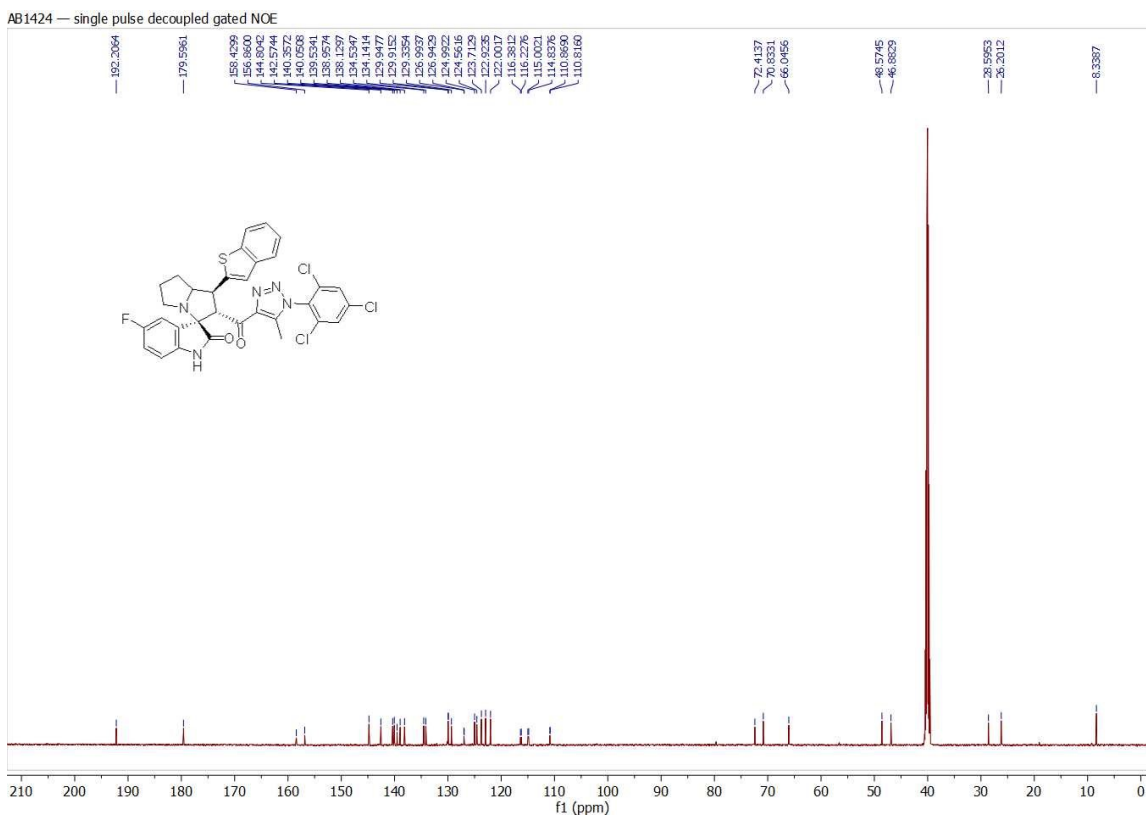


Figure S16: ¹³C NMR (DMSO-*d*₆) for 4f

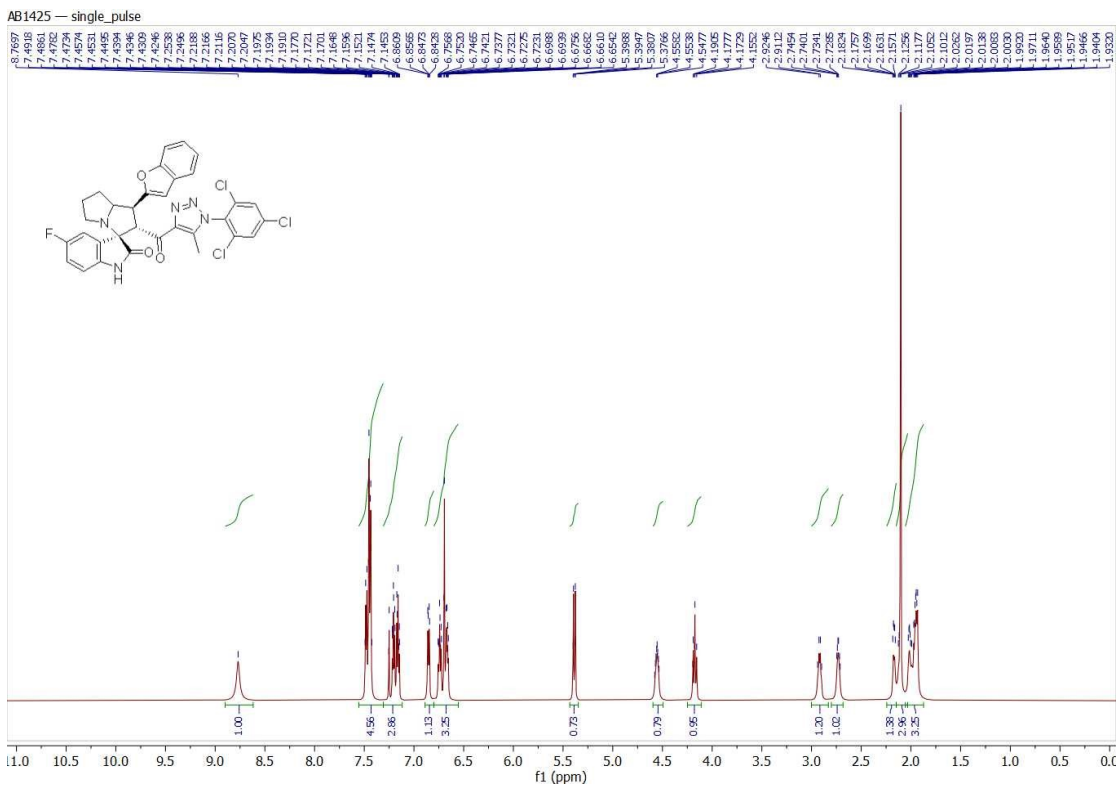


Figure S17: $^1\text{H NMR}$ (CDCl₃) for 4g

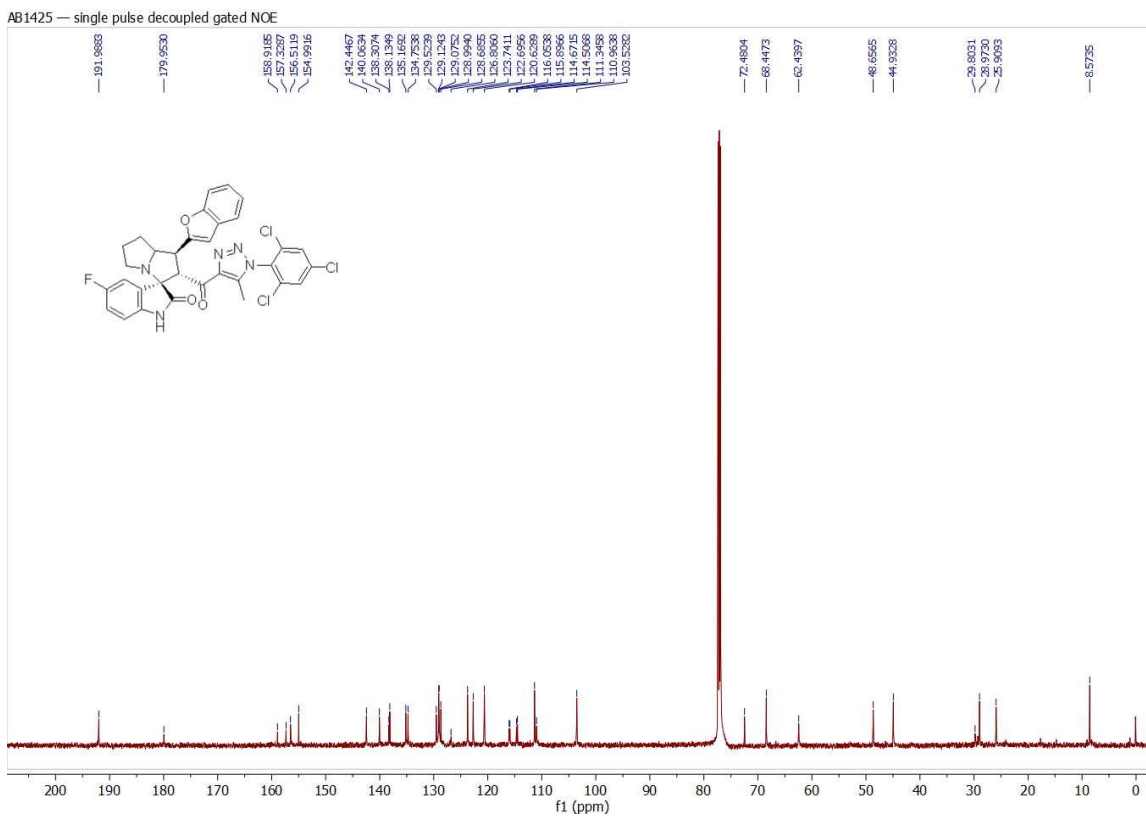


Figure S18: $^{13}\text{C NMR}$ (CDCl₃) for 4g

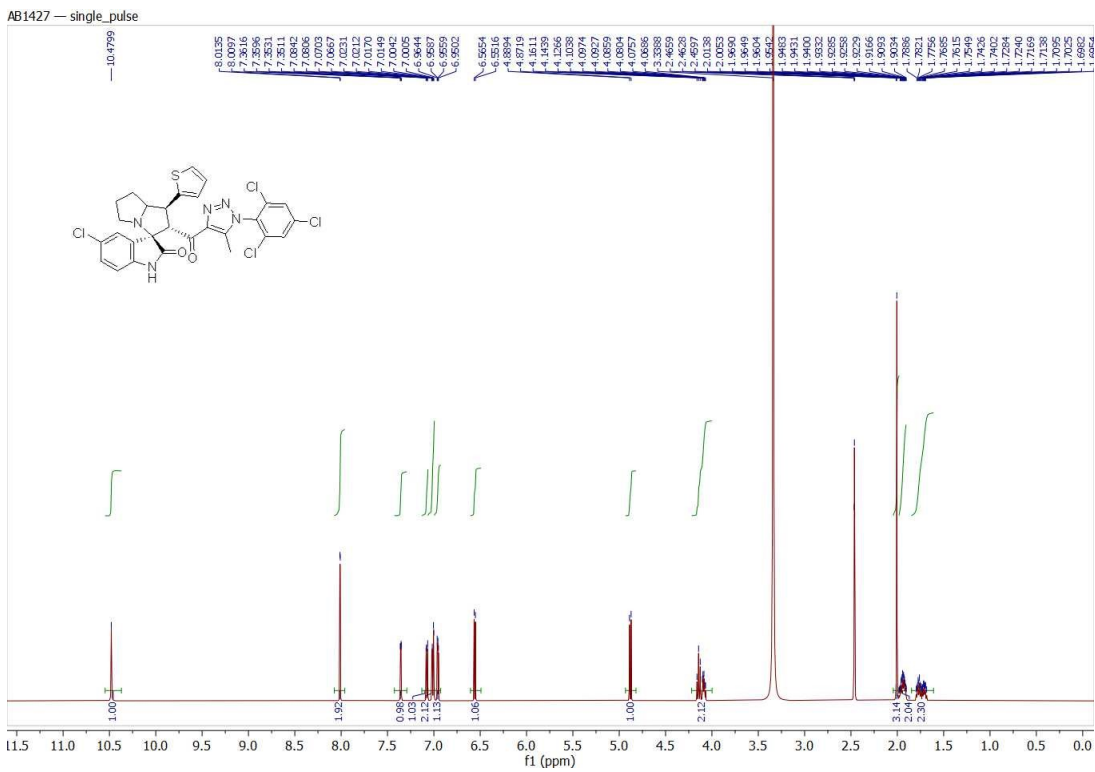


Figure S19: ^1H NMR (DMSO- d_6) for 4i

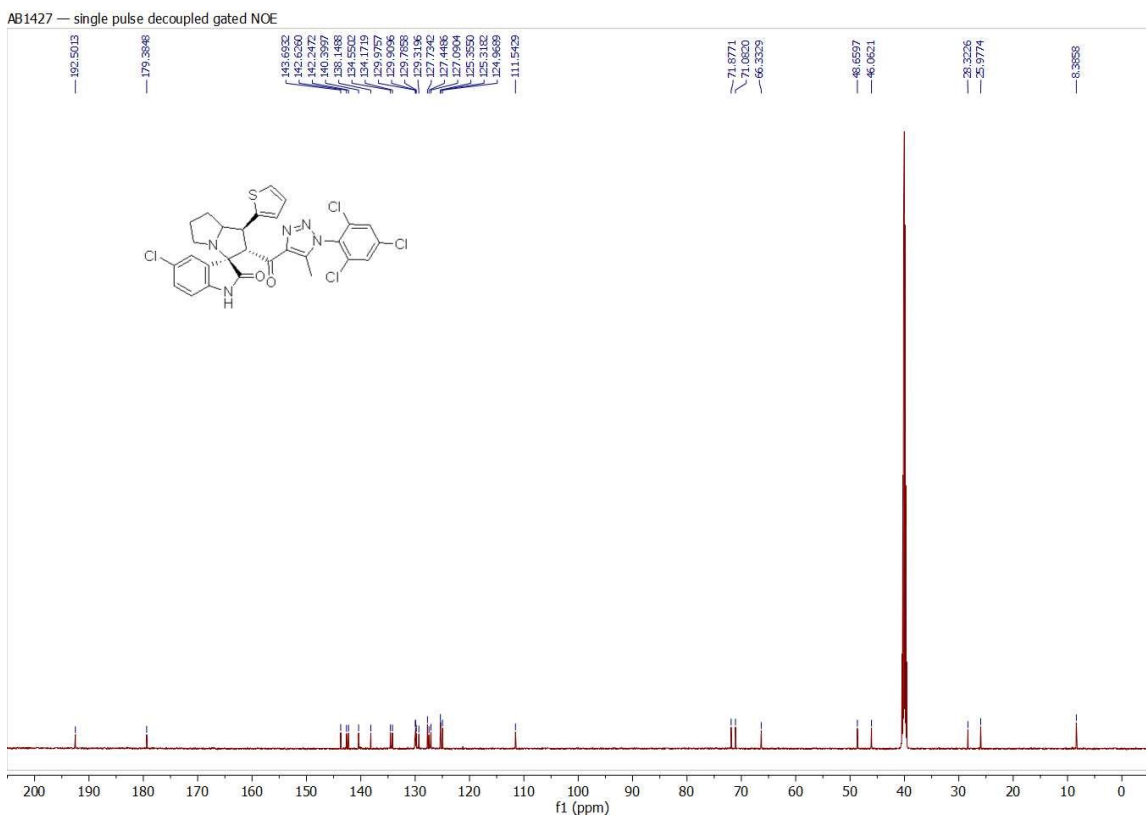


Figure S20: ^{13}C NMR (DMSO- d_6) for 4i

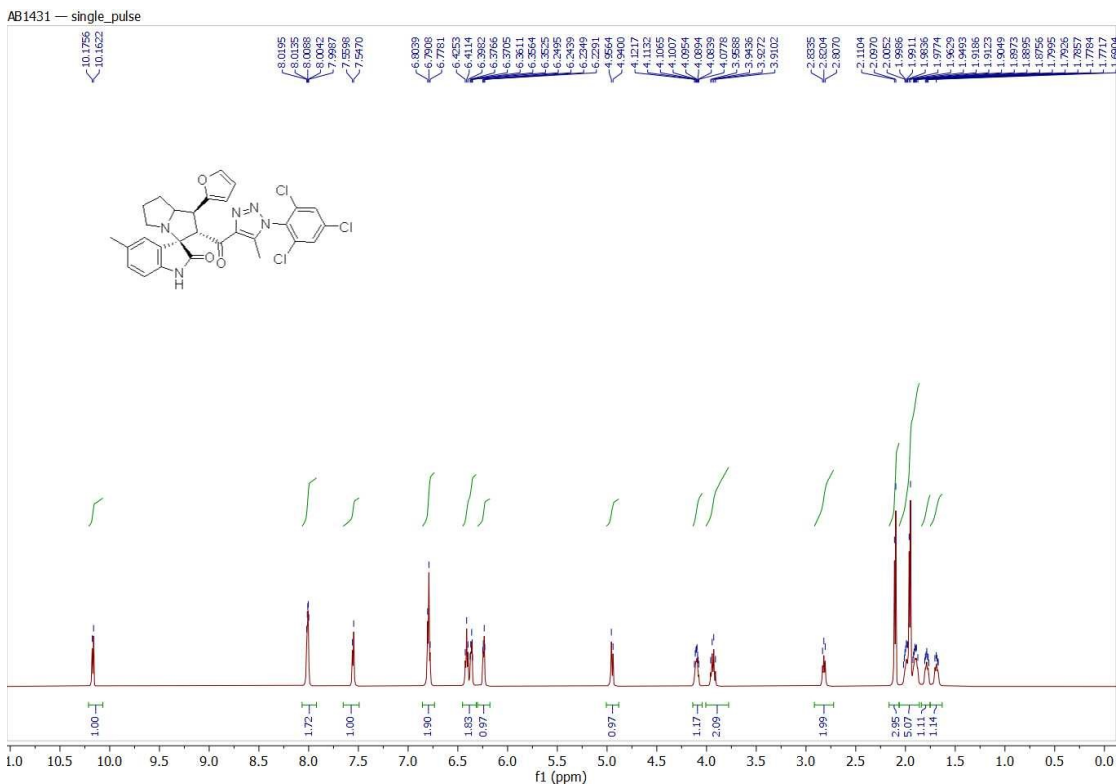


Figure S21: ^1H NMR (DMSO- d_6) for **4j**

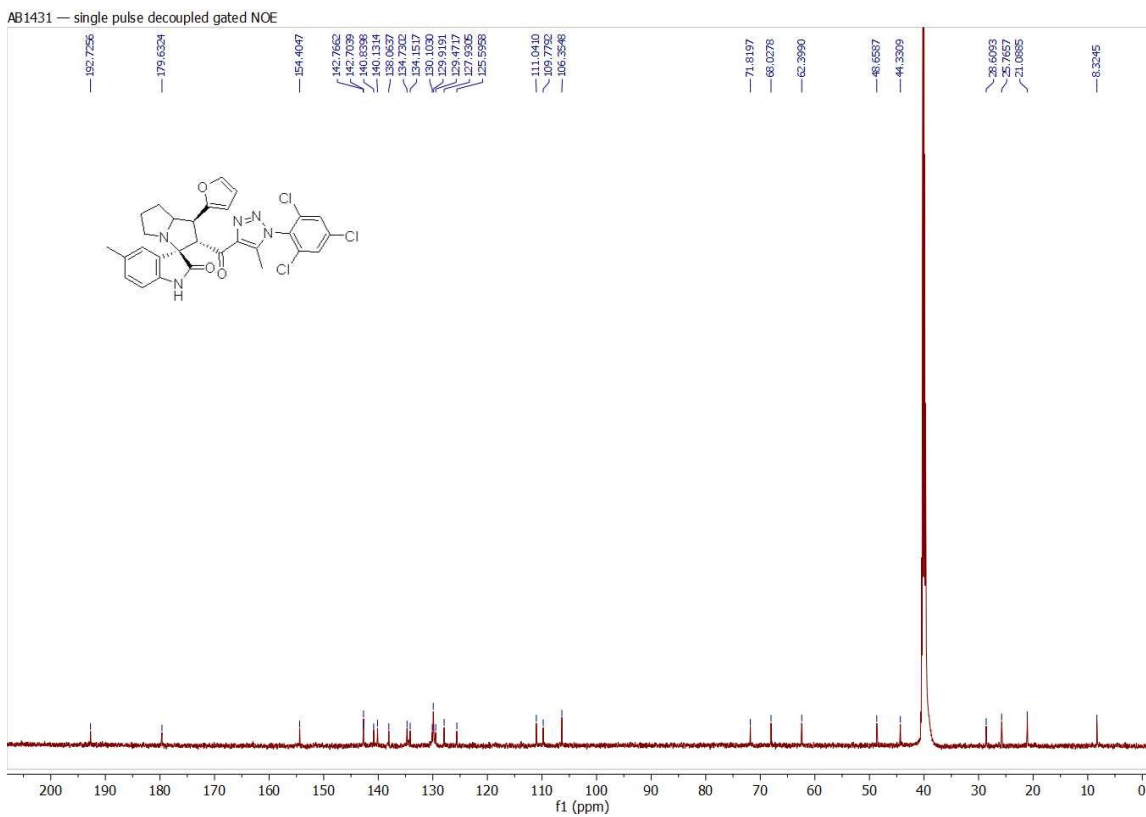


Figure S22: ^{13}C NMR (DMSO- d_6) for **4j**

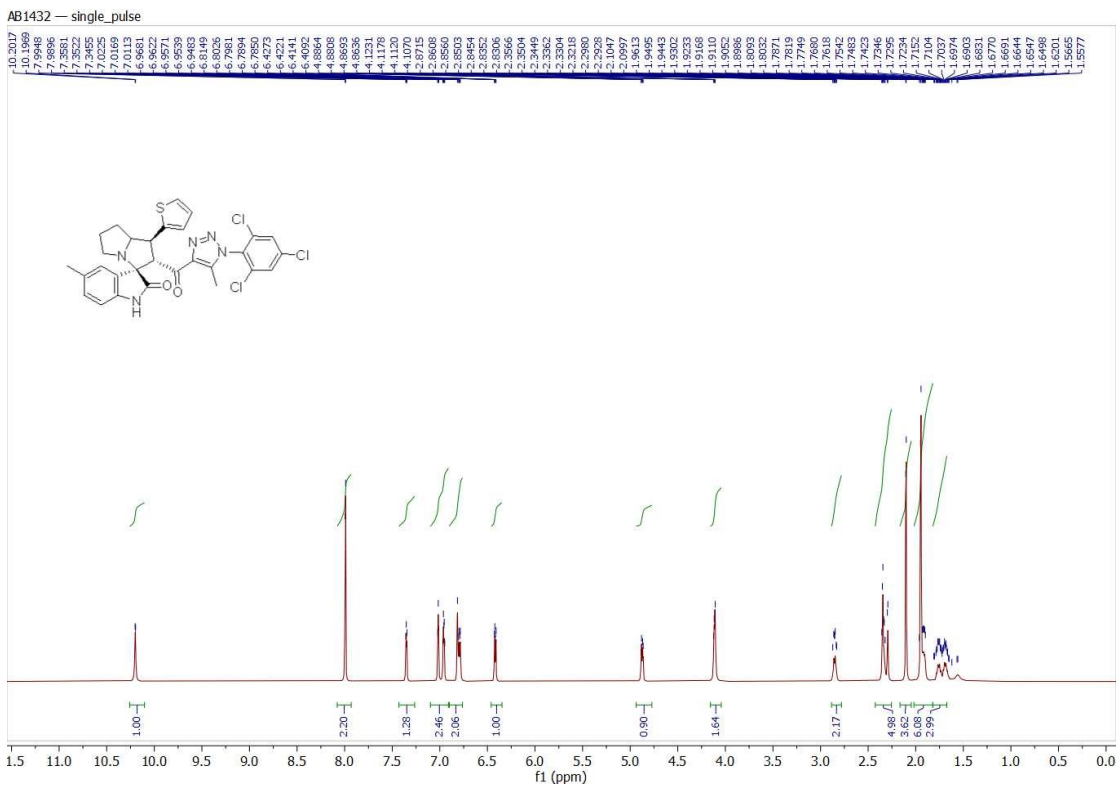


Figure S23: ^1H NMR (DMSO- d_6) for 4k

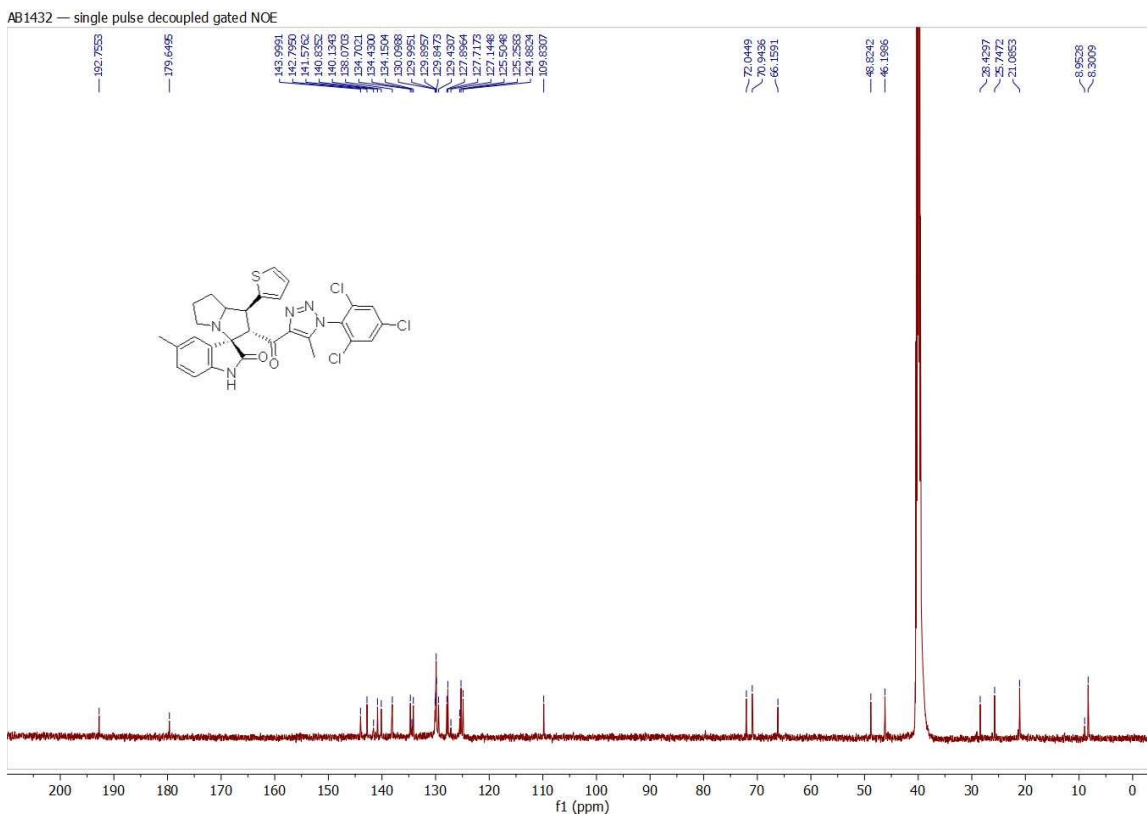


Figure S24: ^{13}C NMR (DMSO- d_6) for 4k

Positive MS Scan 17

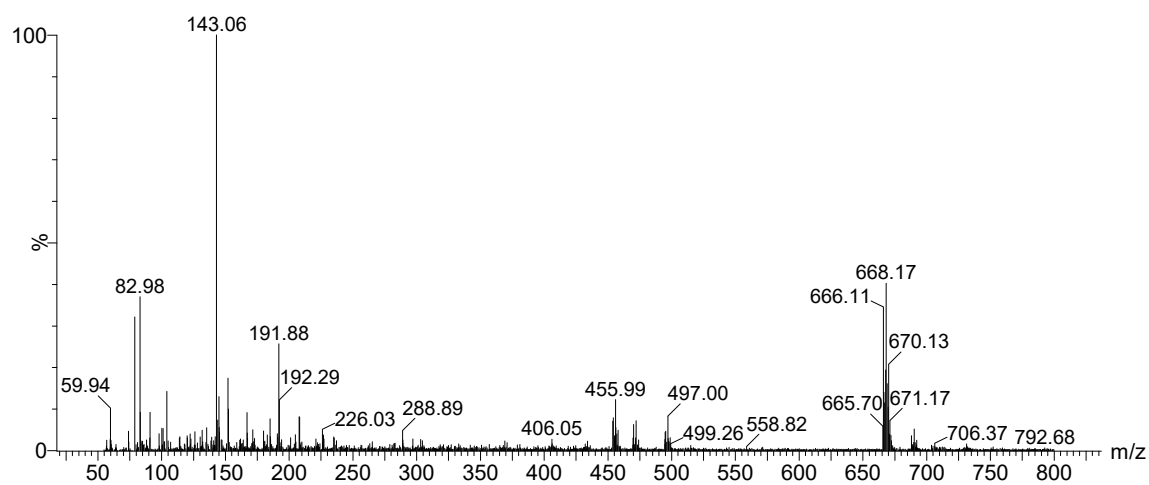


Figure S25: MS for 4a

Positive MS Scan 18

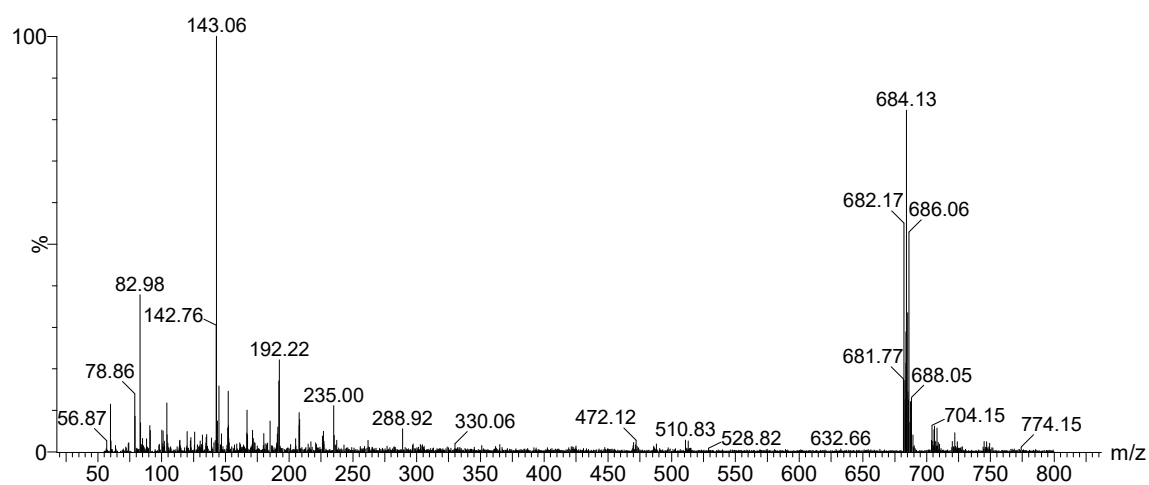


Figure S26: MS for 4b

Positive MS Scan 19

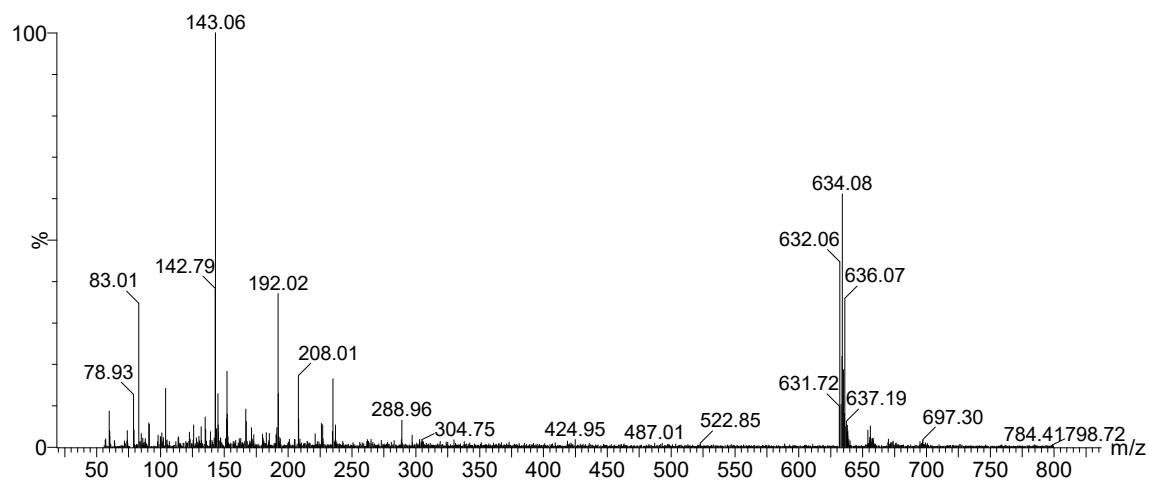


Figure S27: MS for 4c

Positive MS Scan 22

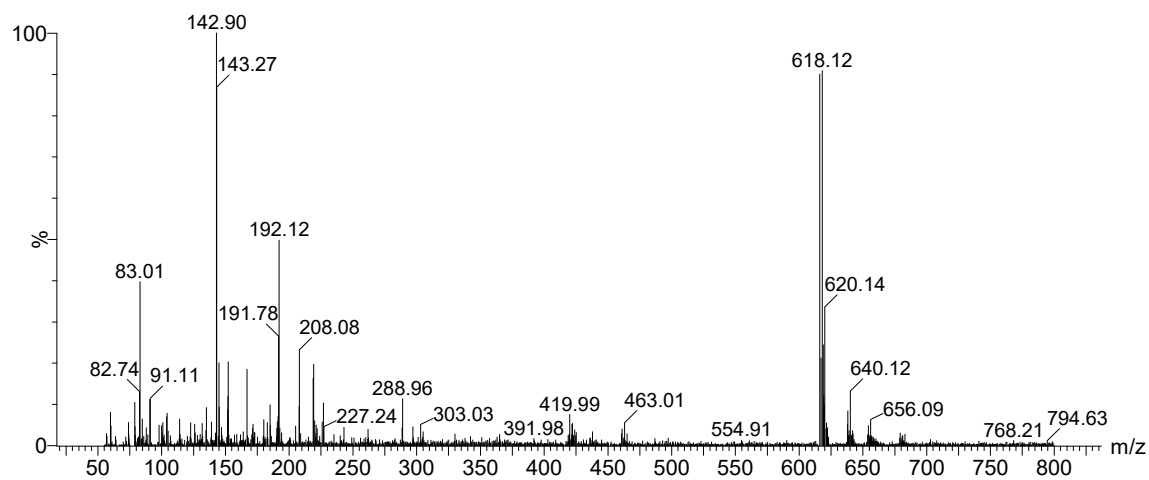


Figure S28: MS for 4d

Positive MS Scan 23

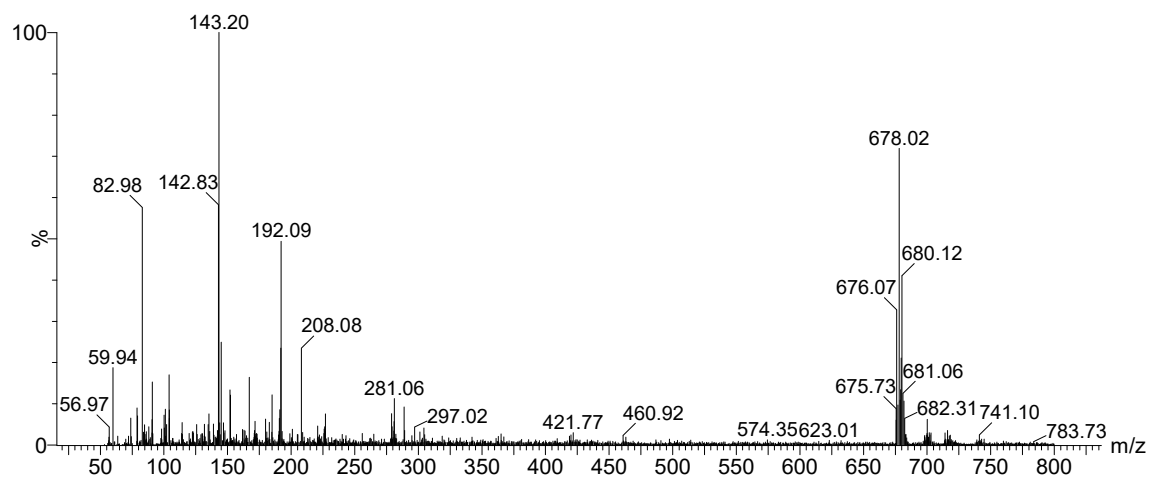


Figure S29: MS for 4e

Positive MS Scan 24

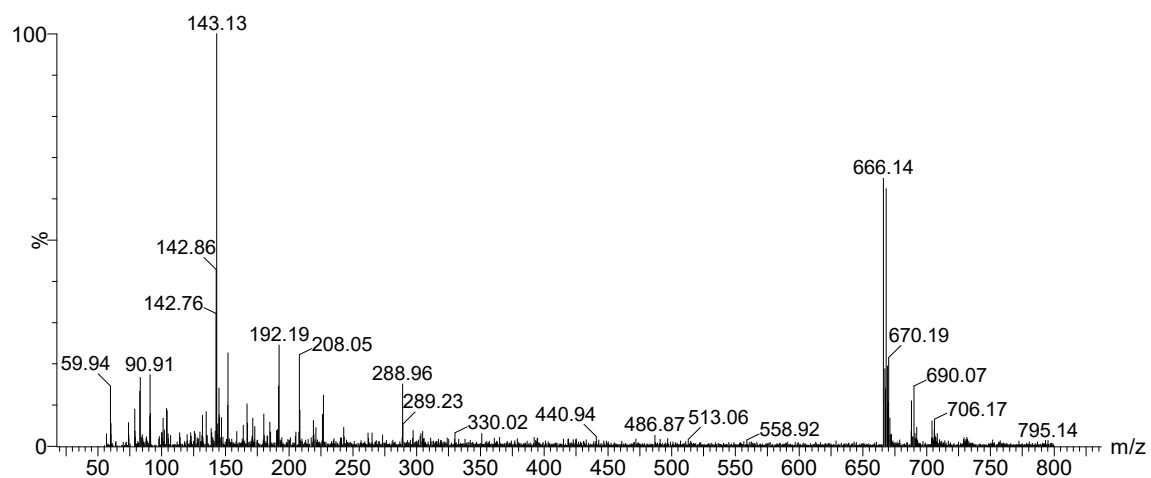


Figure S30: MS for 4f

Positive MS Scan 25

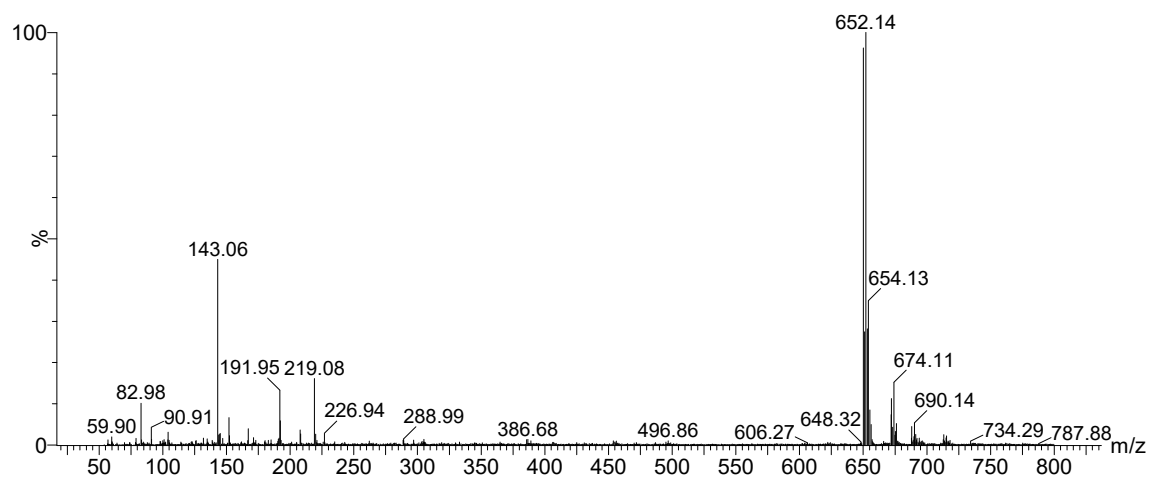


Figure S31: MS for 4g

Positive MS Scan 26

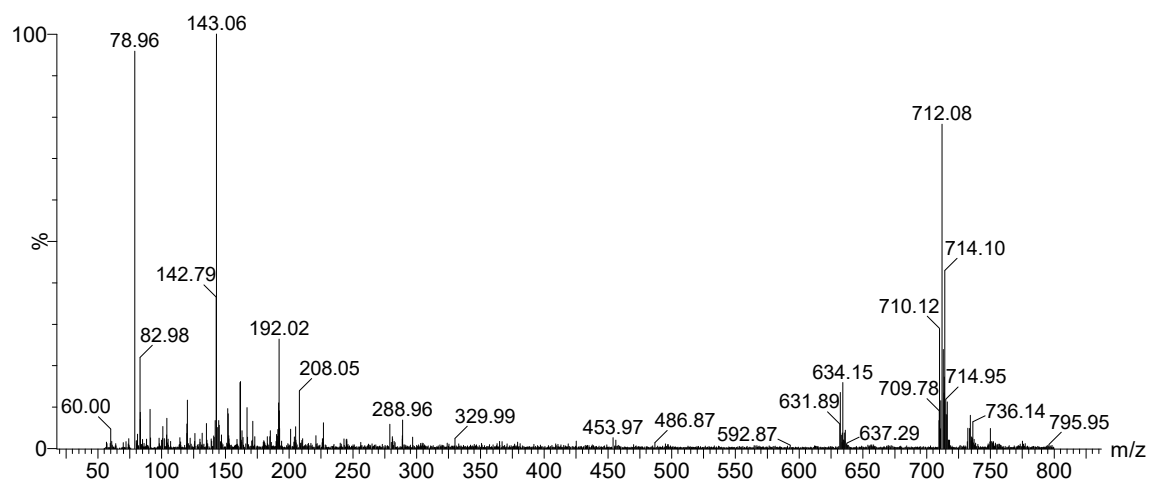


Figure S32: MS for 4h

Positive MS Scan 27

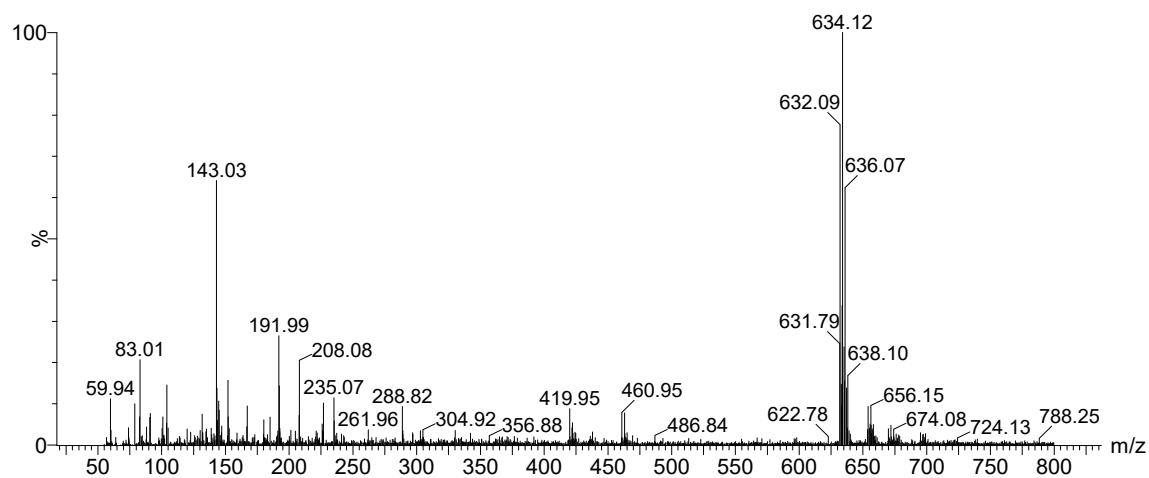


Figure S33: MS for 4i

Positive MS Scan 31

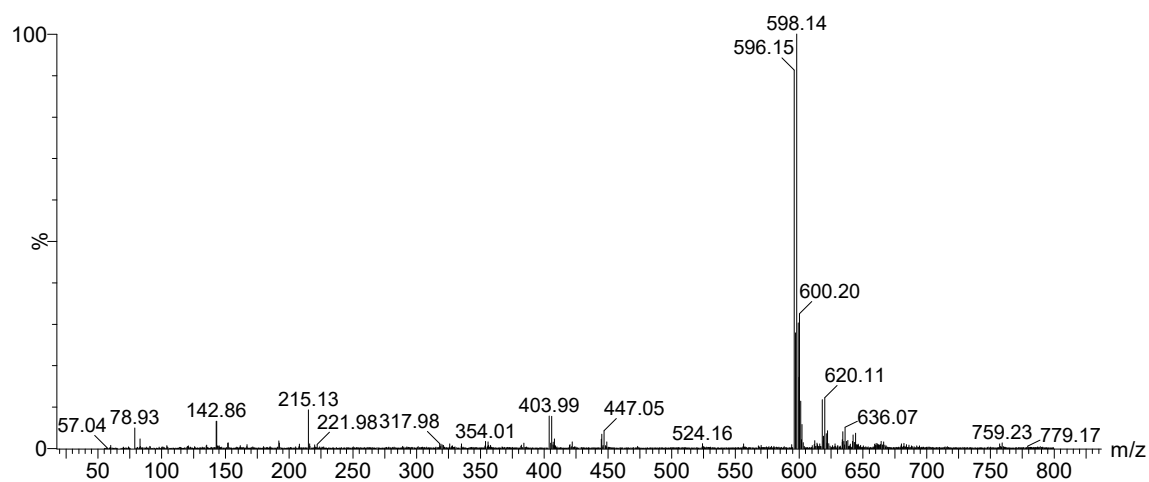


Figure S34: MS for 4j

Positive MS Scan 32

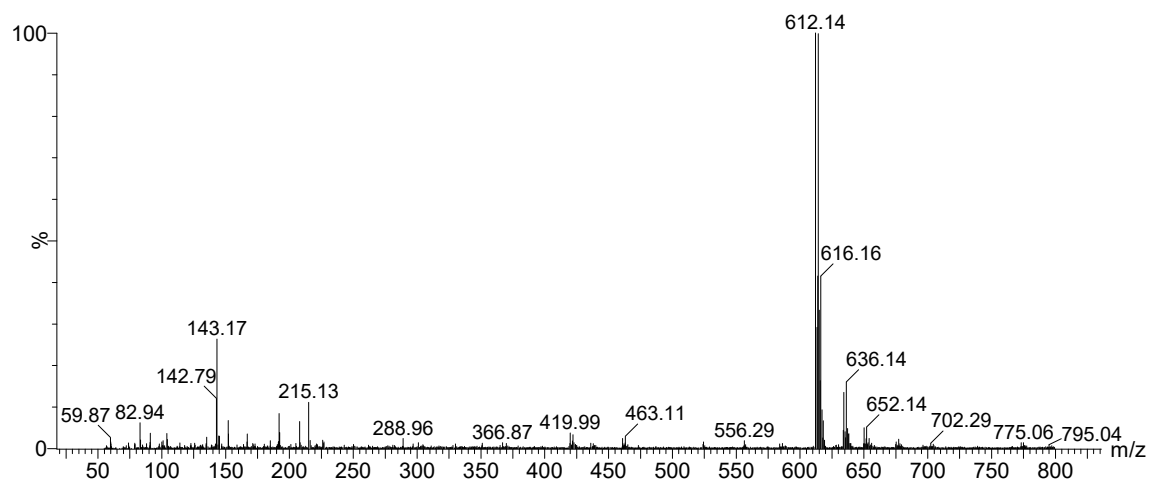


Figure S35: MS for 4k