

Supporting Information

for

An uracil-linked hydroxyflavone probe for the recognition of ATP

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NMR spectra and additional figures

1. NMR spectra of compounds

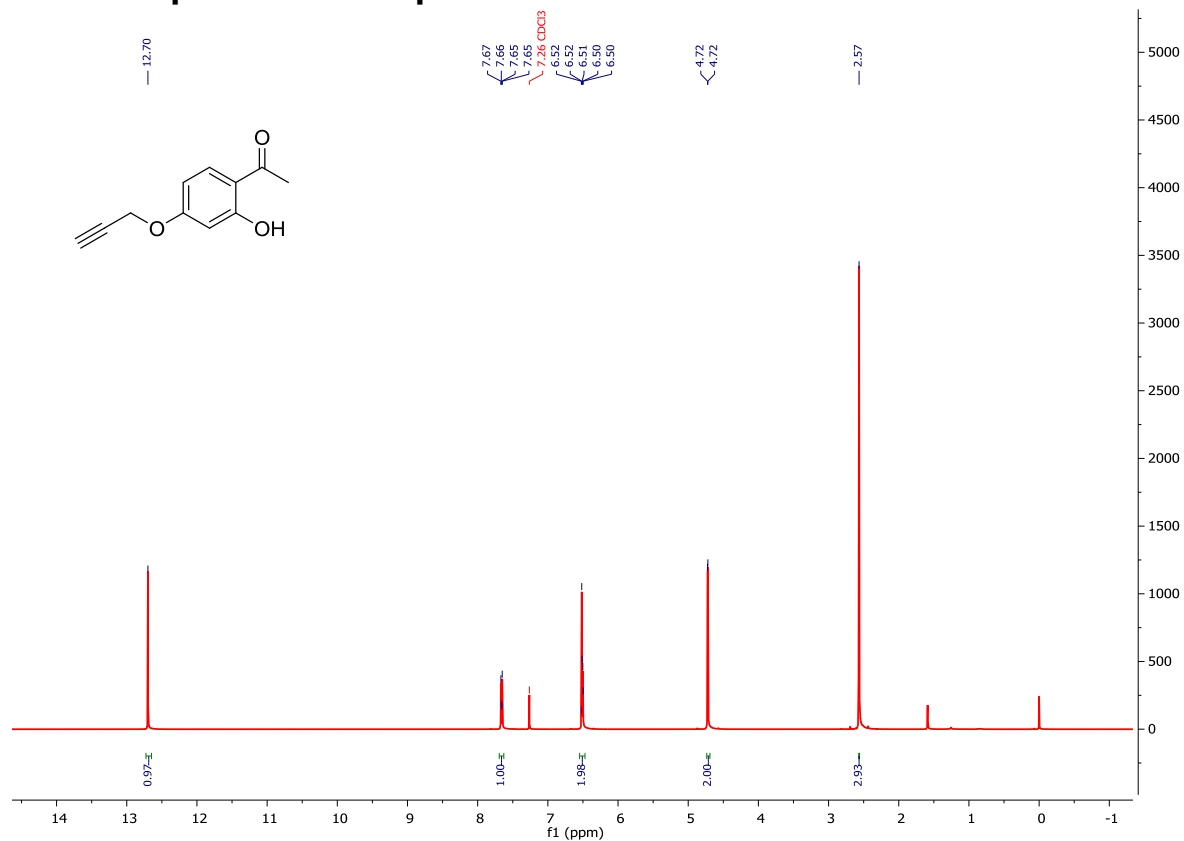


Figure S1: ¹H NMR spectrum of **1** (CDCl₃, 500 MHz, 298 K).

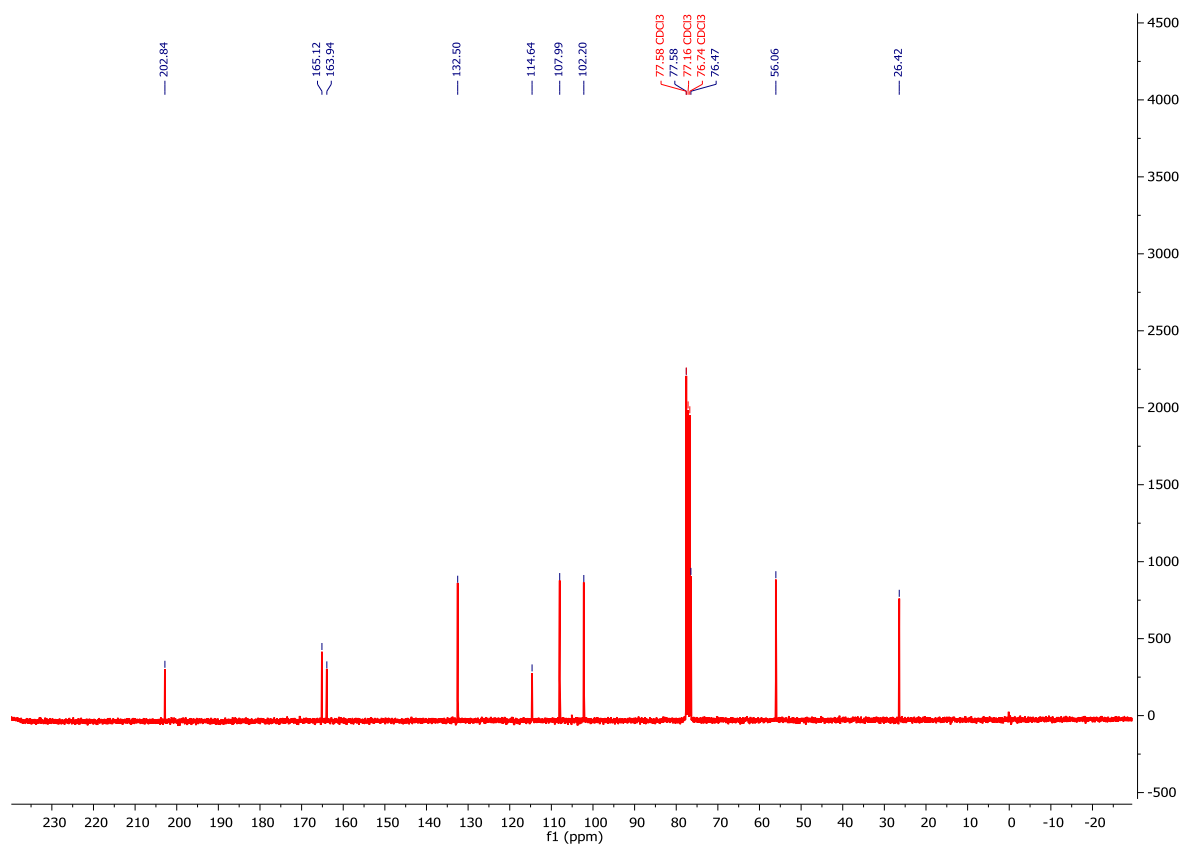


Figure S2: ¹³C NMR spectrum of **1** (CDCl₃, 75 MHz, 298 K).

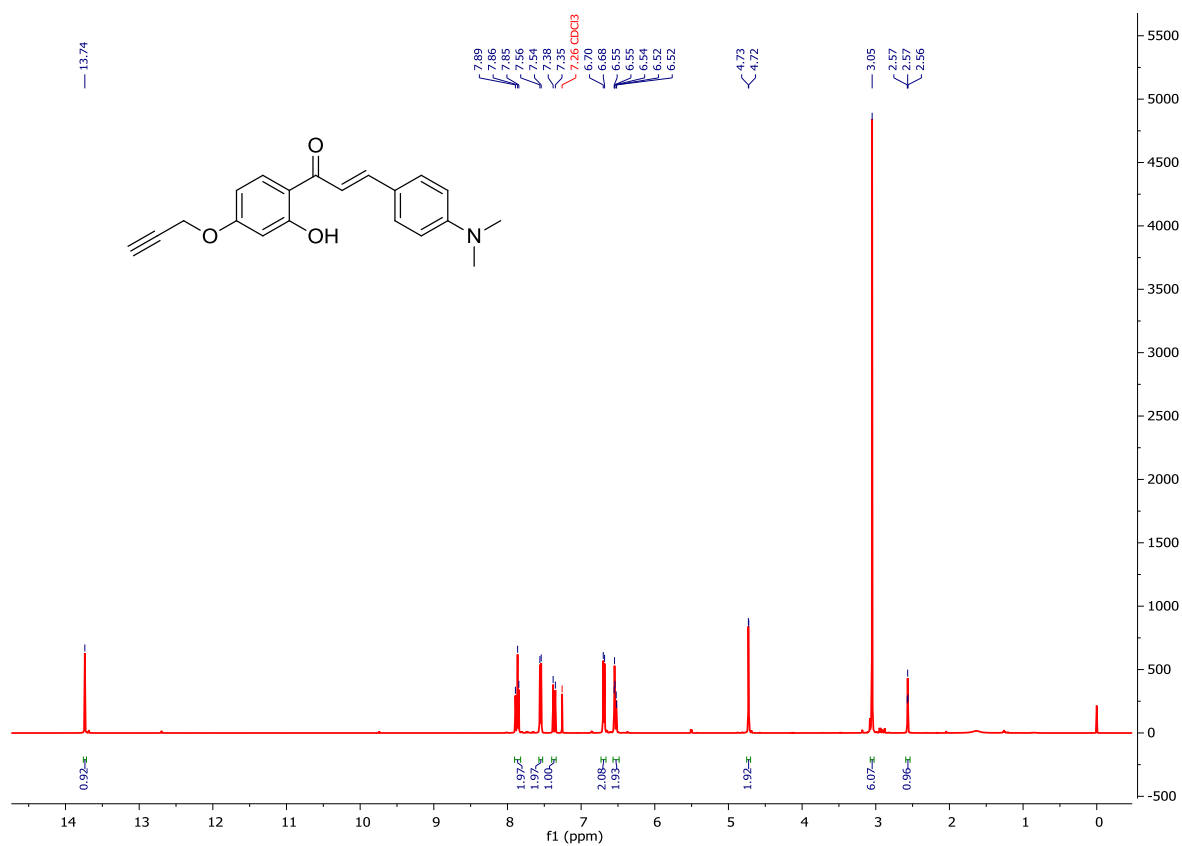


Figure S3: ¹H NMR spectrum of **2** (CDCl₃, 500 MHz, 298 K).



Figure S4: ¹³C NMR spectrum of **2** (CDCl₃, 126 MHz, 298 K).

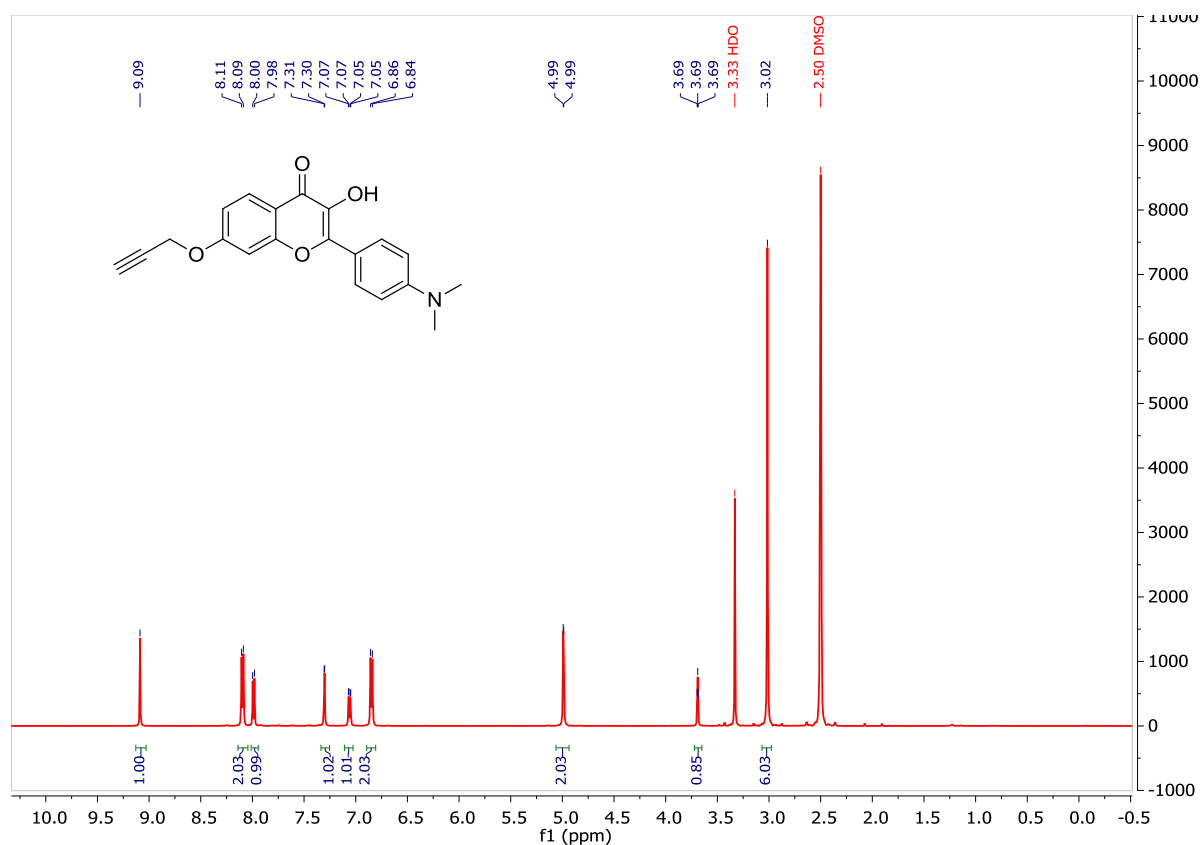


Figure S5: ¹H NMR spectrum of **3** (DMSO, 500 MHz, 298 K).

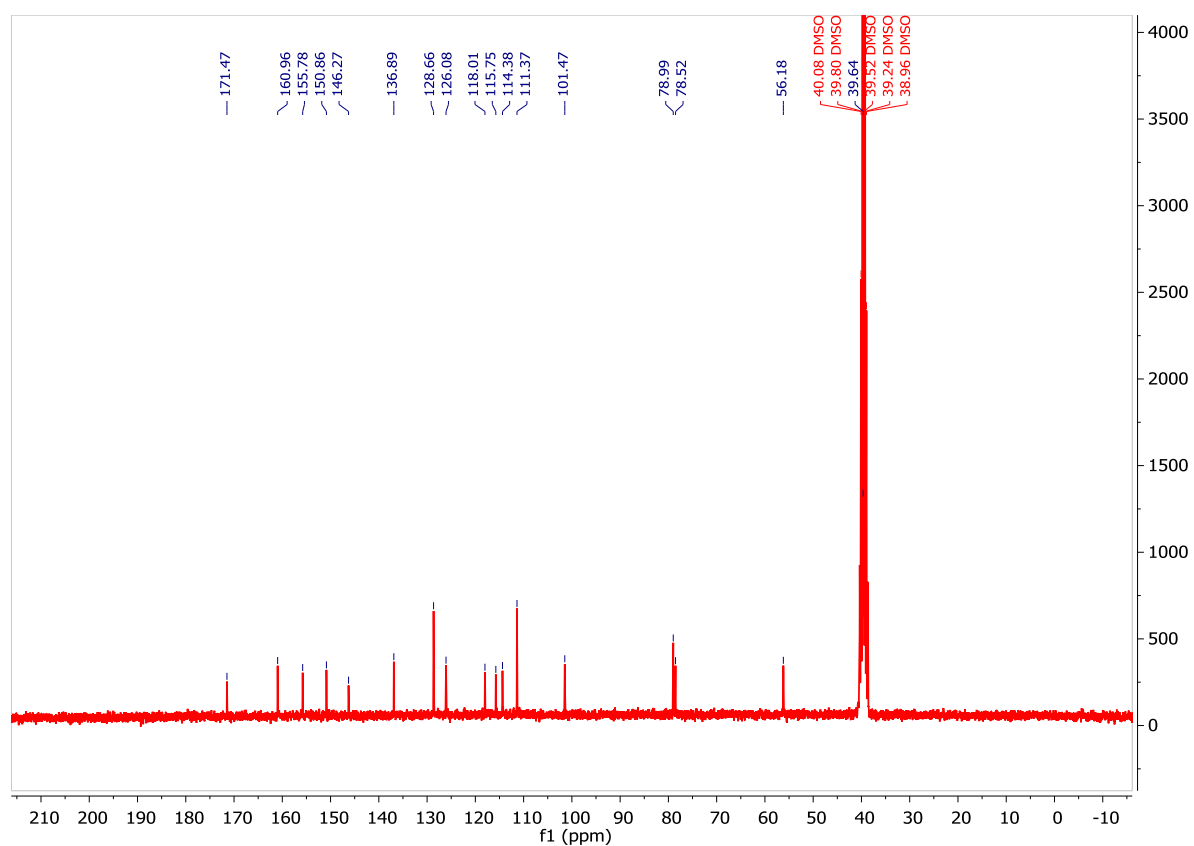


Figure S6: ¹³C NMR spectrum of **3** (DMSO, 75 MHz, 298 K).

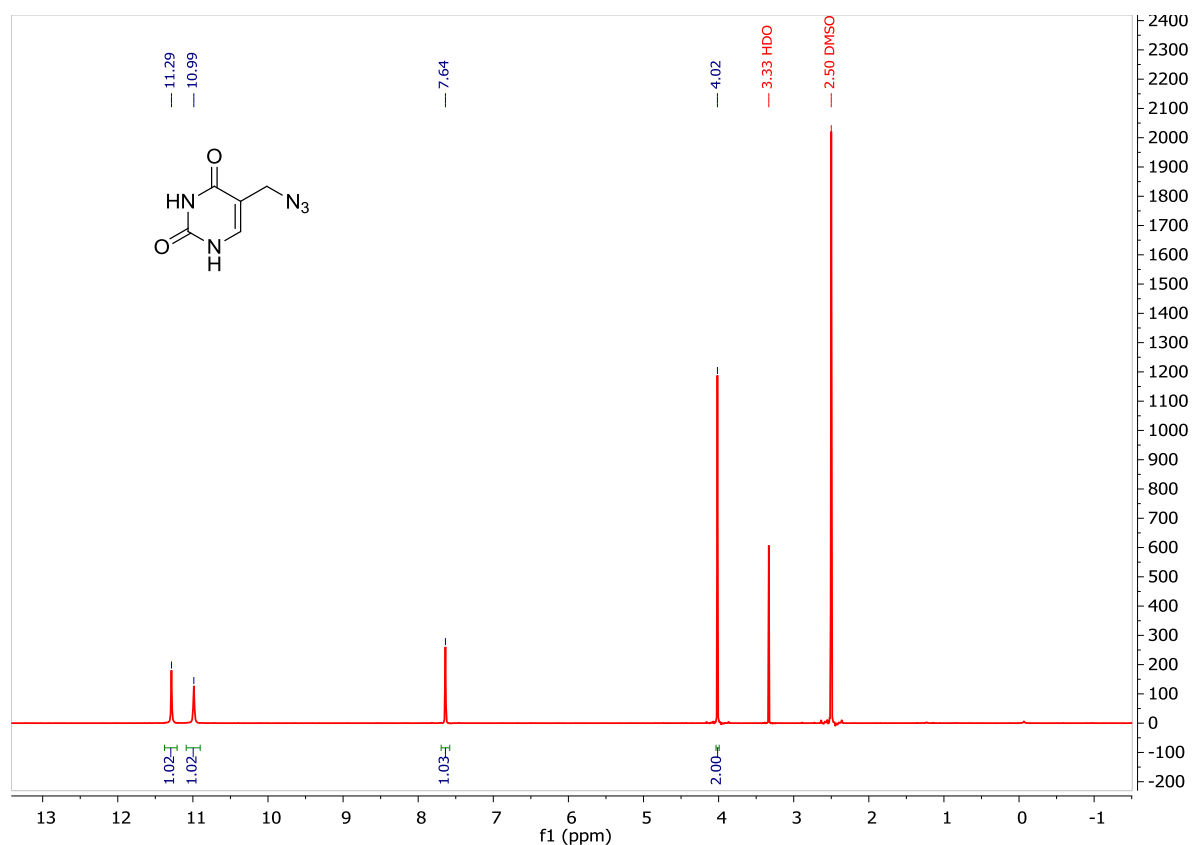


Figure S7: ^1H NMR spectrum of **4** (DMSO, 500 MHz, 298 K).

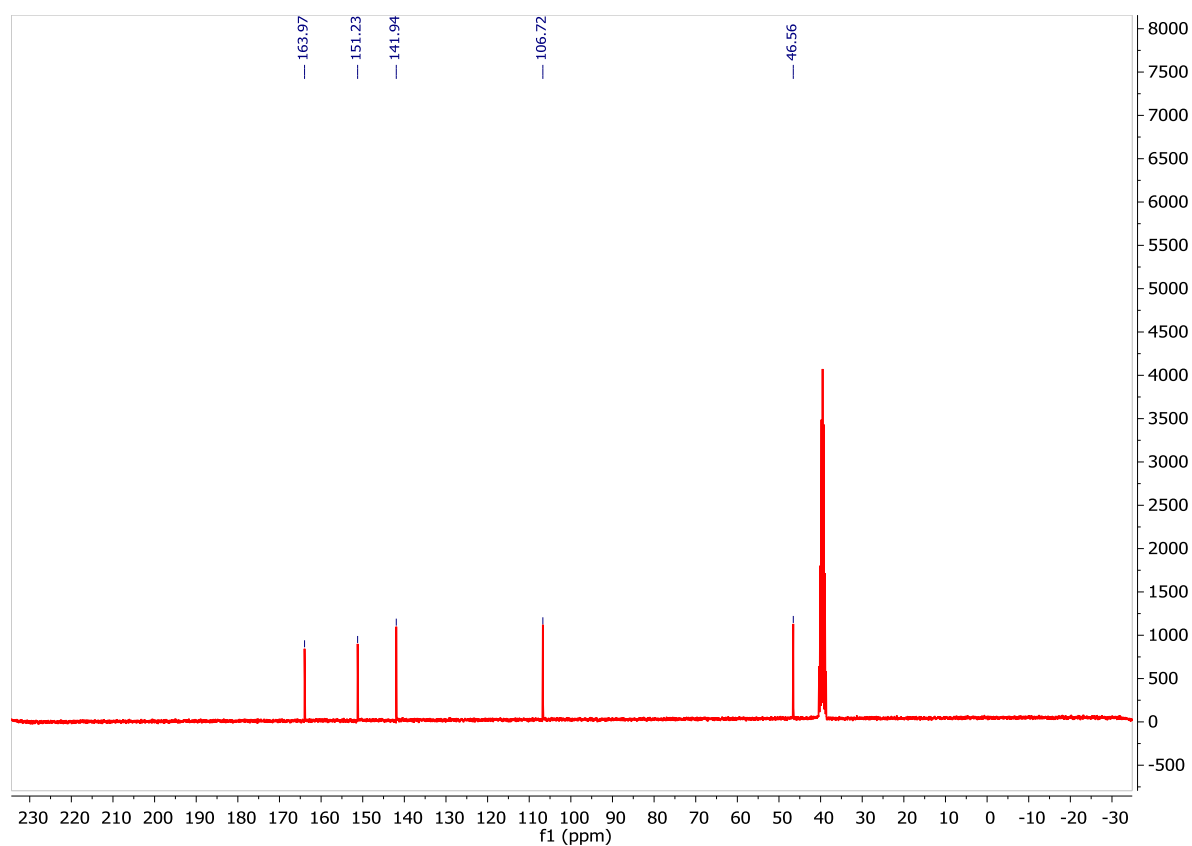


Figure S8: ^{13}C NMR spectrum of **4** (DMSO, 75 MHz, 298 K).

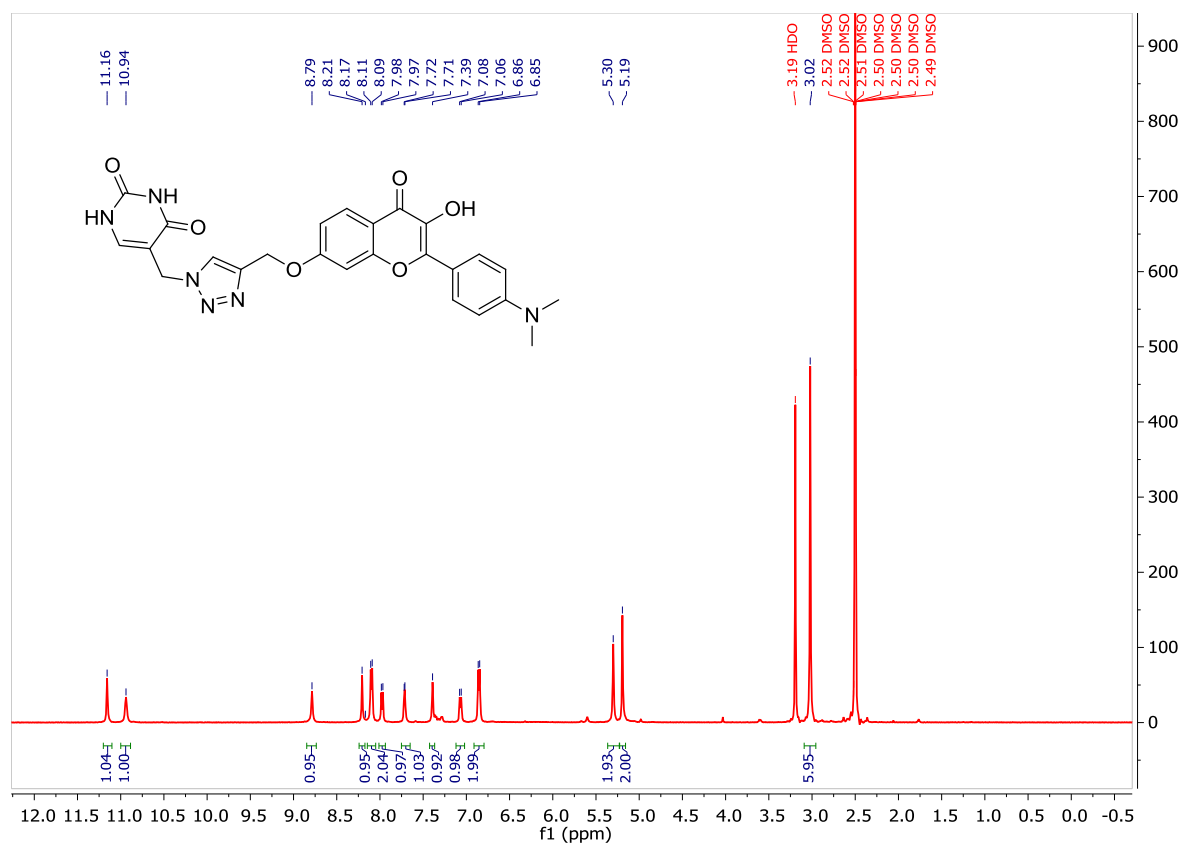


Figure S9: ¹H NMR spectrum of UHF (DMSO, 500 MHz, 298 K).

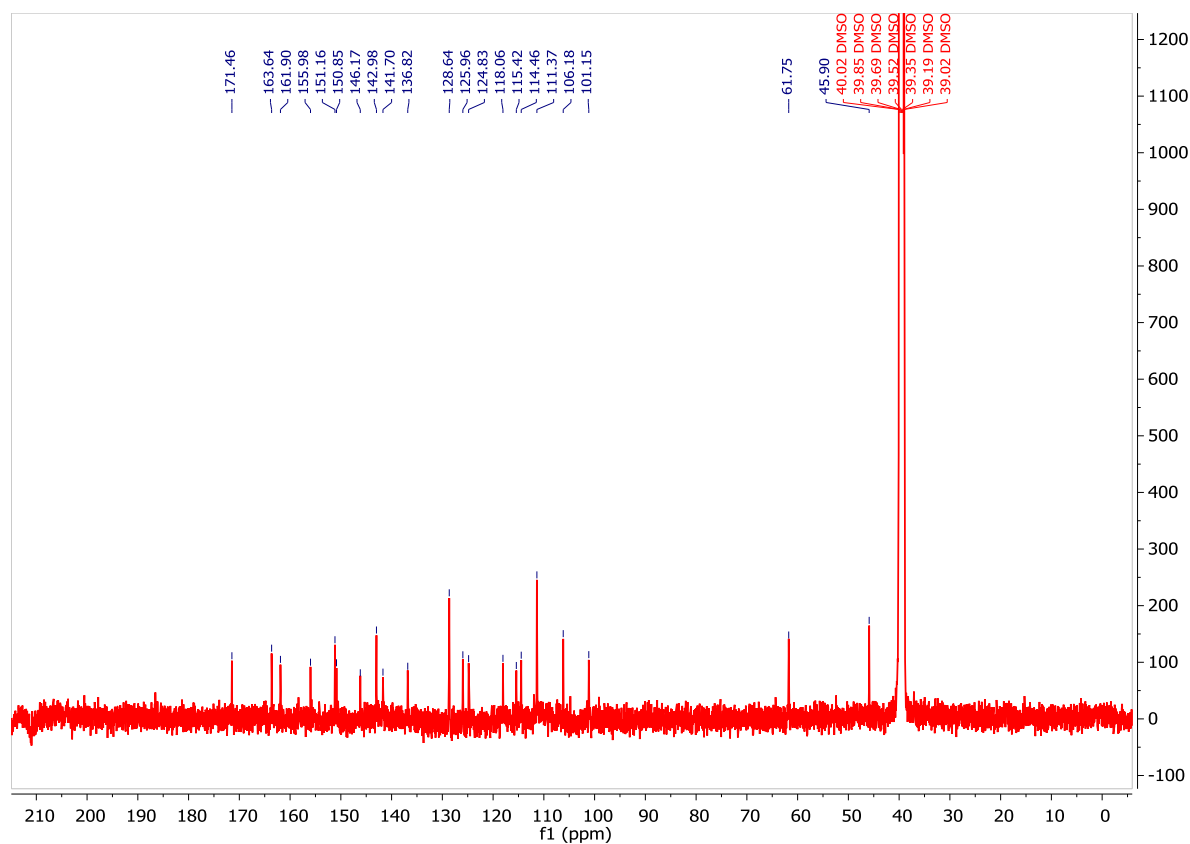


Figure S10: ¹³C NMR spectrum of UHF (DMSO, 126 MHz, 298 K).

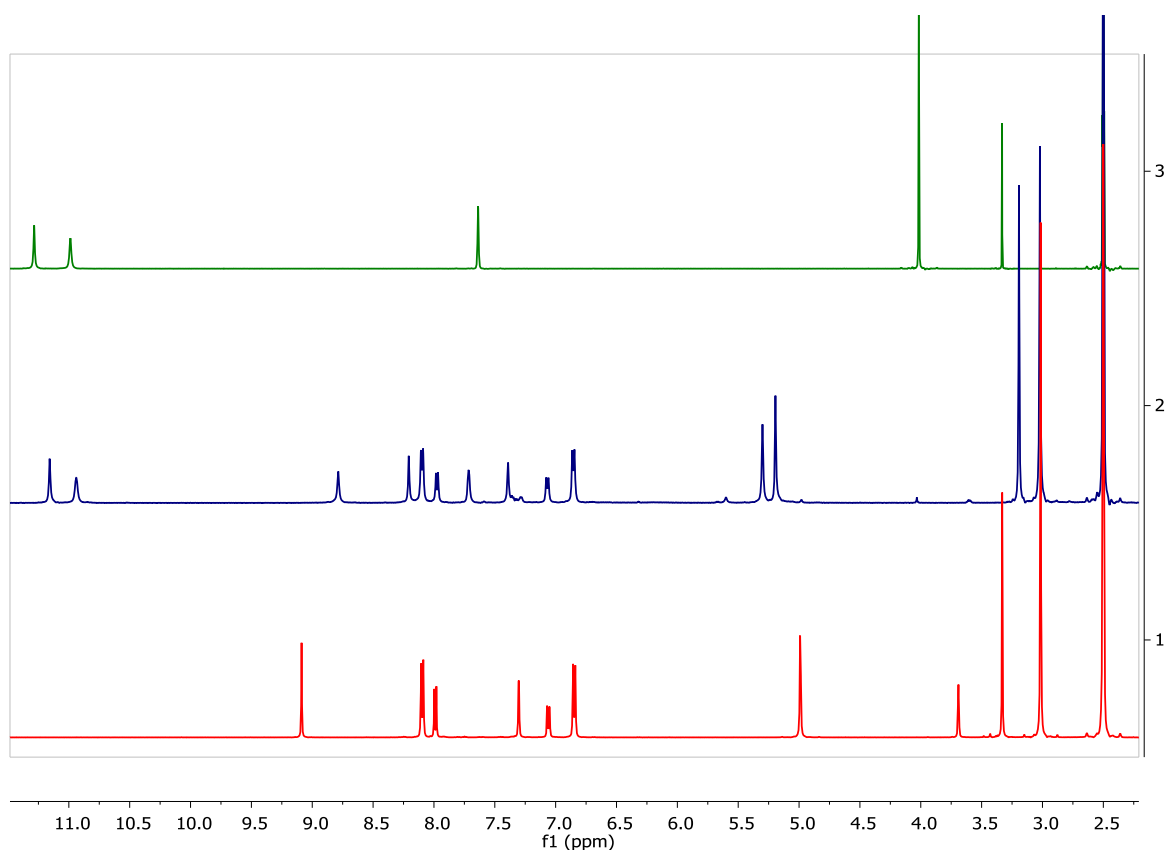


Figure S11: Stacked ^1H NMR spectra of (top) **4** (middle) **UHF** (bottom) **3** (DMSO, 500 MHz, 298 K) for the assignment of the protons before and after the click reaction.

2. HRMS data of compounds

User Spectra

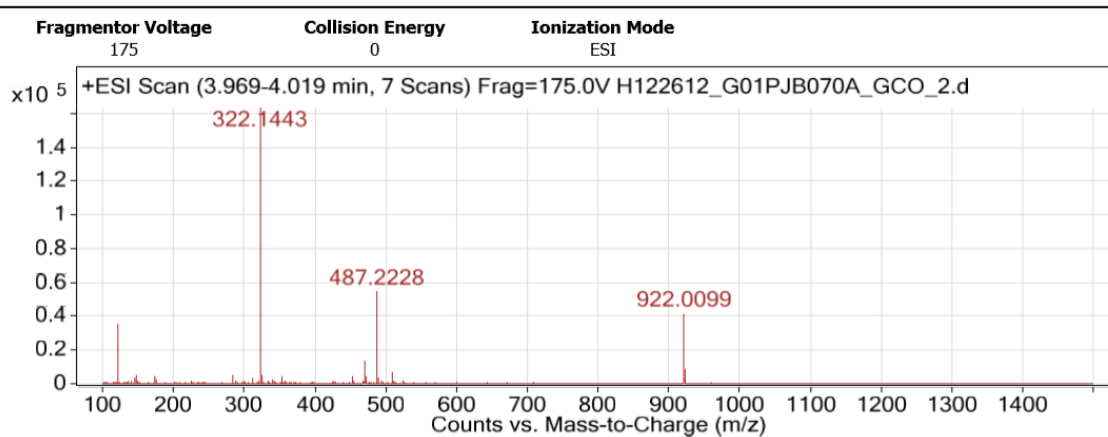


Figure S12: HRMS spectrum of **2**. Calculated mass for $[\text{M} + \text{H}]^+$: 322.1443

User Spectra

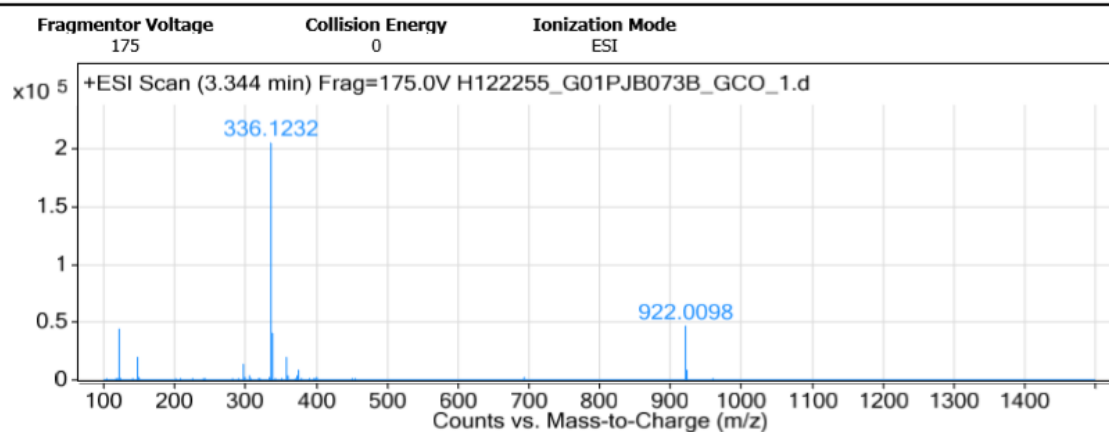


Figure S13: HRMS spectrum of **3**. Calculated mass for $[M + H]^+$: 336.1236

User Spectra

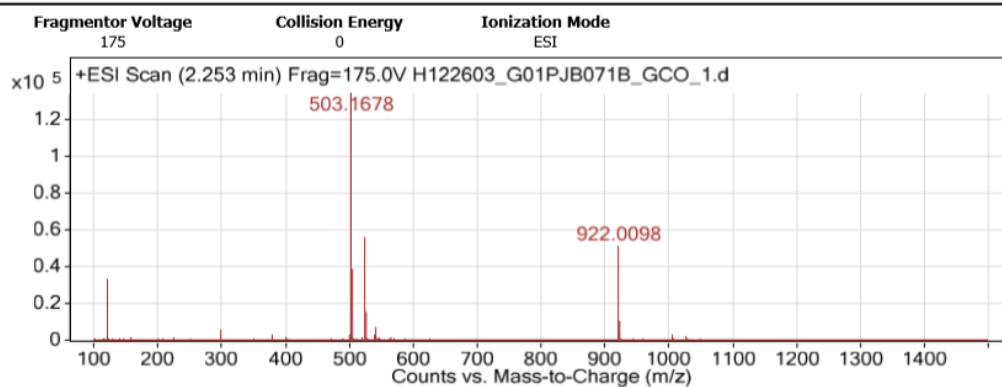


Figure S14: HRMS spectrum of **UHF**. Calculated mass for $[M + H]^+$: 503.1679

Note: HRMS data for **1** and **4** can be found in the literature ([1,2]).

3. Absorption spectra

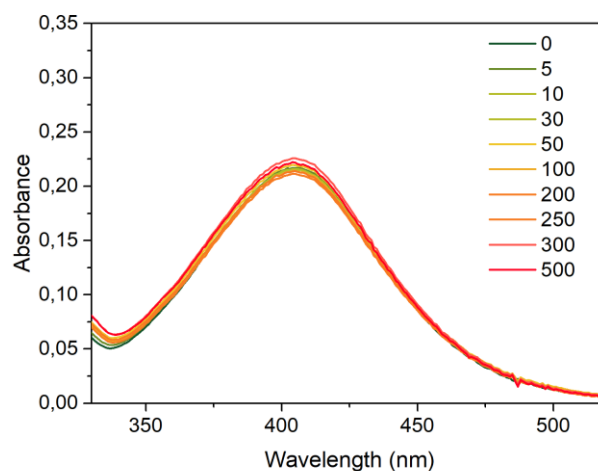


Figure S15: UV–vis spectra of UHF (1.0 μM) upon addition of increasing amount of ATP in 0.02 M HEPES which also contains 0.1 mM γ -cyclodextrin using a cuvette with a path length of 10 cm. The ATP equivalents to the probe are shown on the graph.

References

1. Anand, N.; Singh, P.; Sharma, A.; Tiwari, S.; Singh, V.; Singh, D. K.; Srivastava, K. K.; Singh, B. N.; Tripathi, R. P. *Bioorg. Med. Chem.* **2012**, *20*, 5150–5163.
doi:10.1016/j.bmc.2012.07.009
2. Nguyen, K.; Fazio, M.; Kubota, M.; Nainar, S.; Feng, C.; Li, X.; Atwood, S. X.; Bredy, T. W.; Spitale, R. C. *J. Am. Chem. Soc.* **2017**, *139*, 2148–2151.
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