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Supplementary Information

STING antagonists, synthesized via Povarov-Doebner type multicomponent reaction

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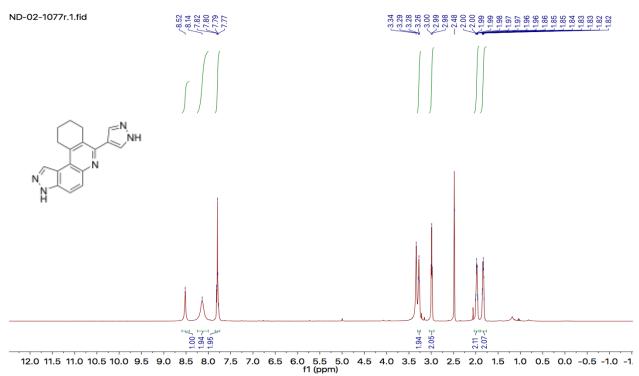
^c Purdue Institute of Inflammation, Immunology, and Infectious Disease, West Lafayette, IN, 47907, USA

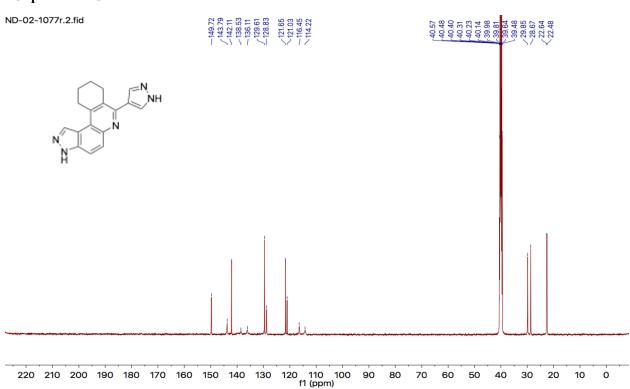
*Corresponding author. Email: hsintim@purdue.edu

- I. ¹H and ¹³C Spectra of compounds
- II. HPLC Purity Chromatograms
- III. Full blots of Western used in the paper

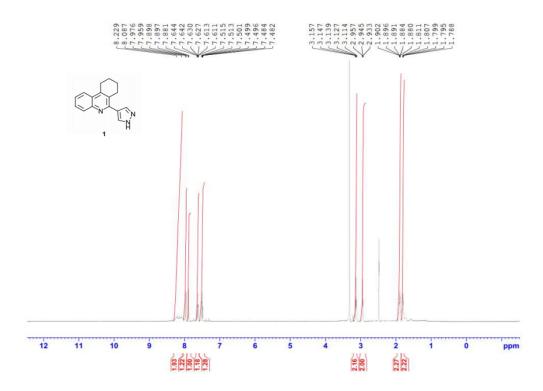
I. ¹H and ¹³C Spectra of compounds

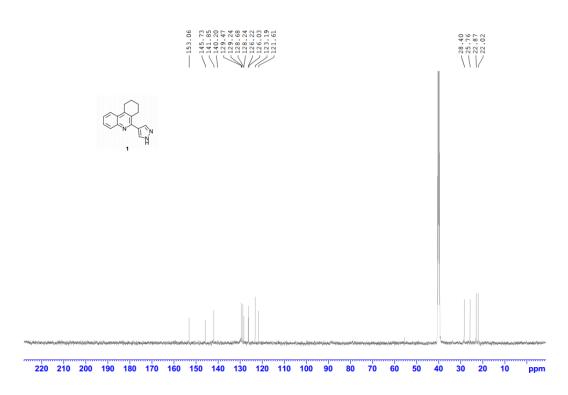
¹H spectra of HSD1077



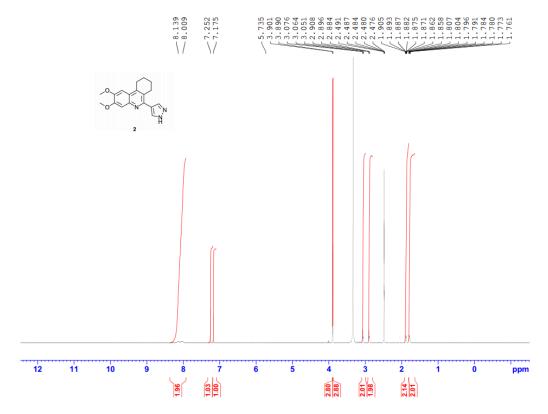


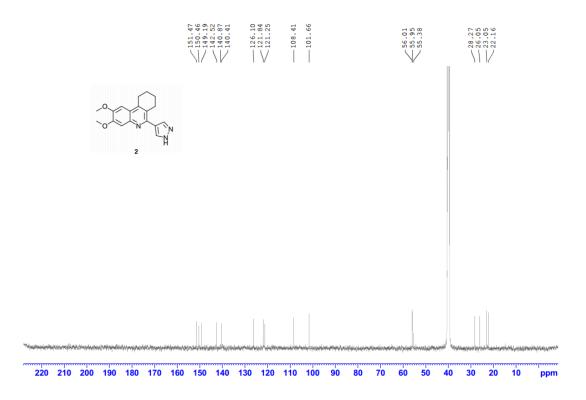
¹H spectra of 1



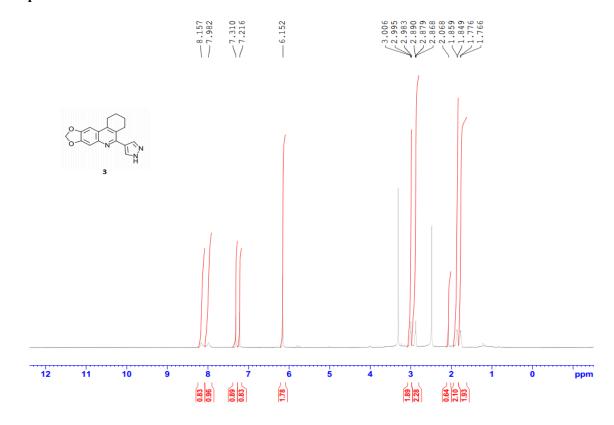


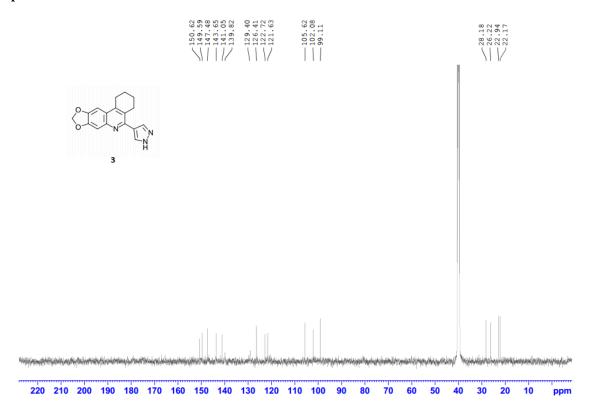
¹H spectra of 2

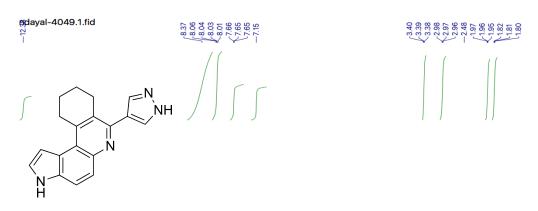


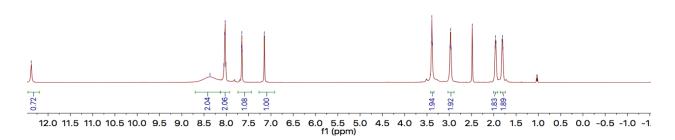


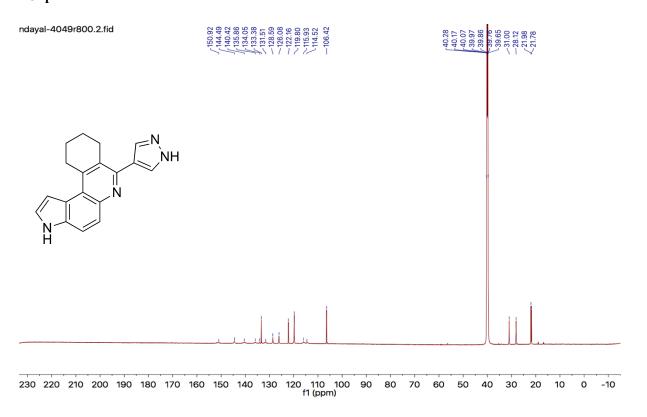
¹H spectra of 3

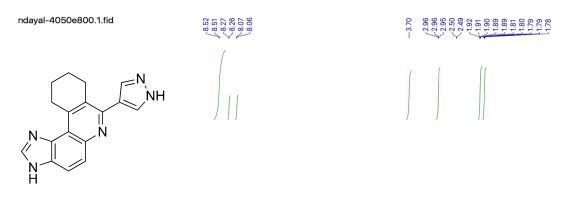


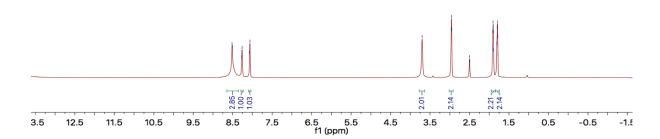


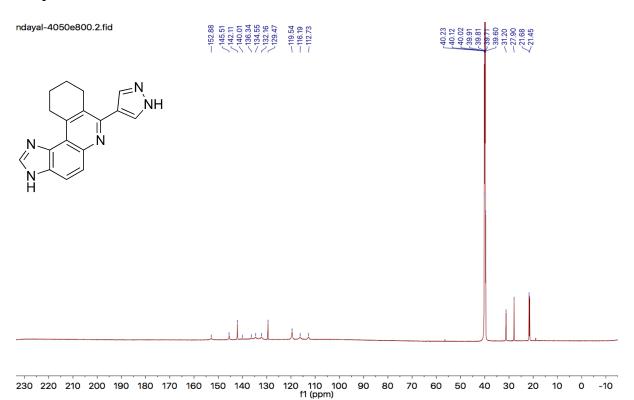




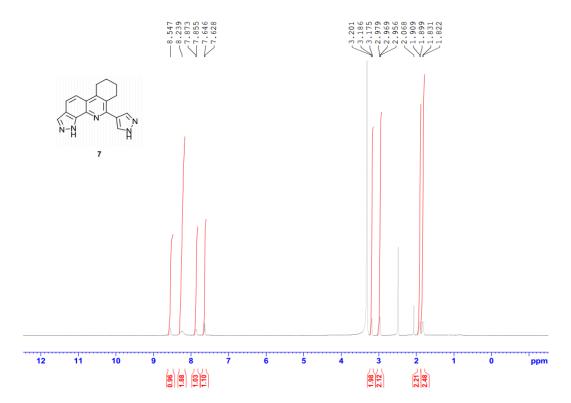




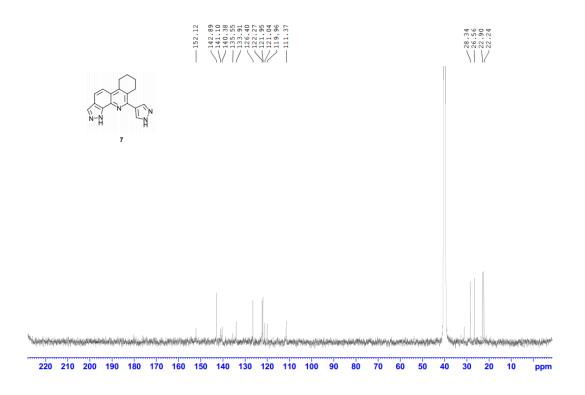




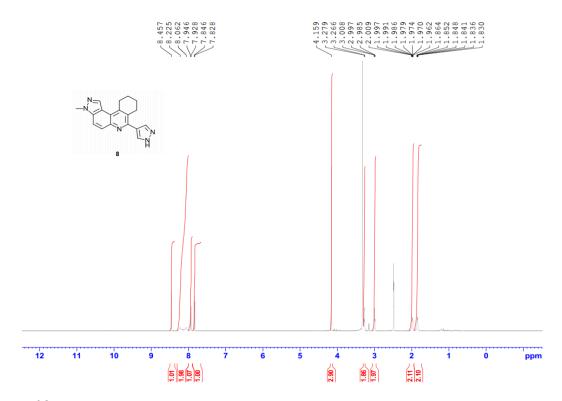
¹H spectra of 7



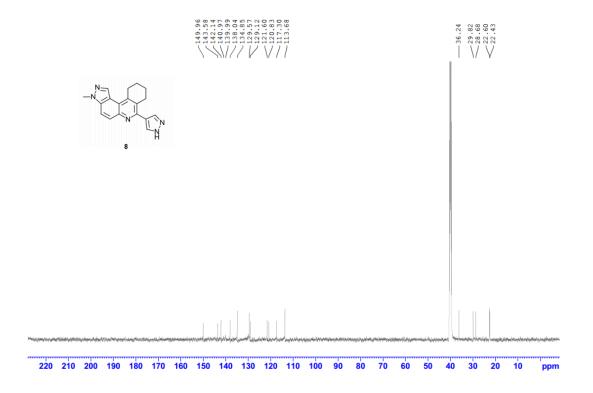
¹³C spectra of 7



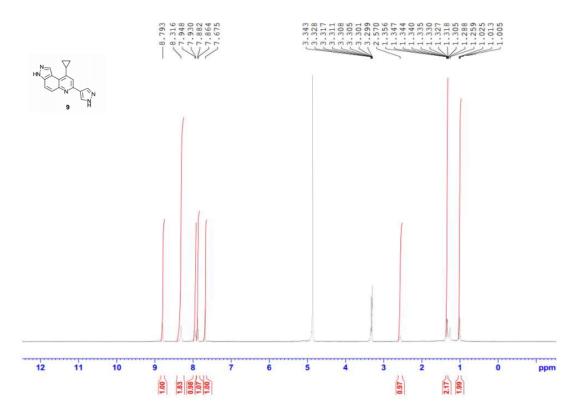
¹H spectra of 8

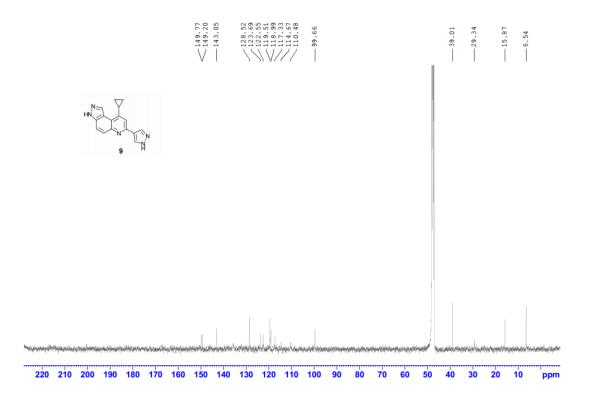


¹³C spectra of 8

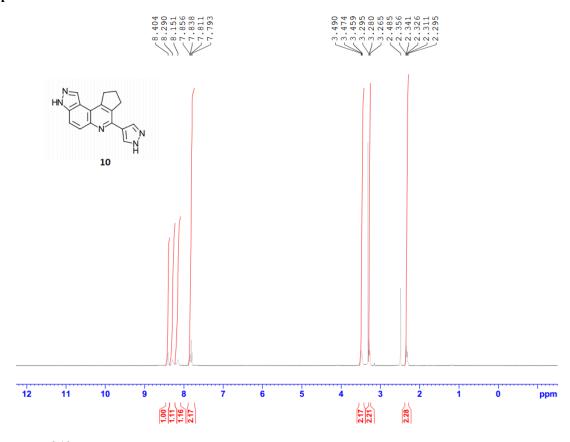


¹H spectra of 9

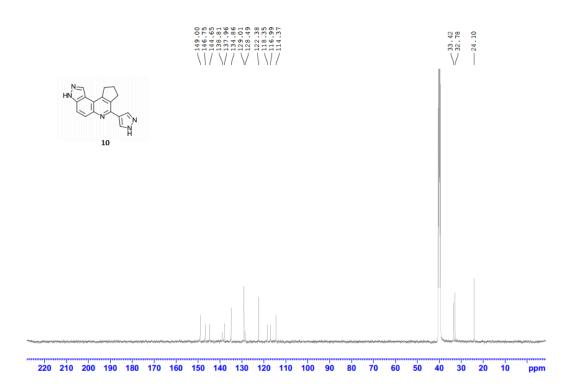




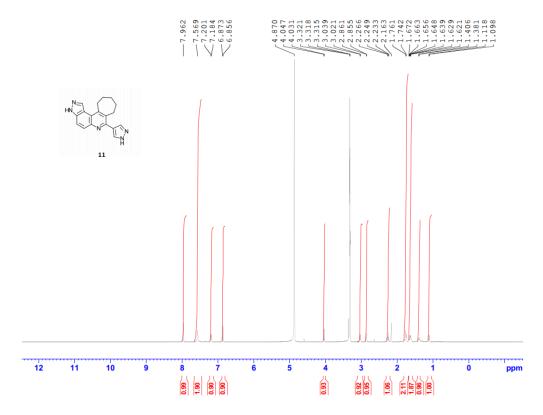
¹H spectra of 10

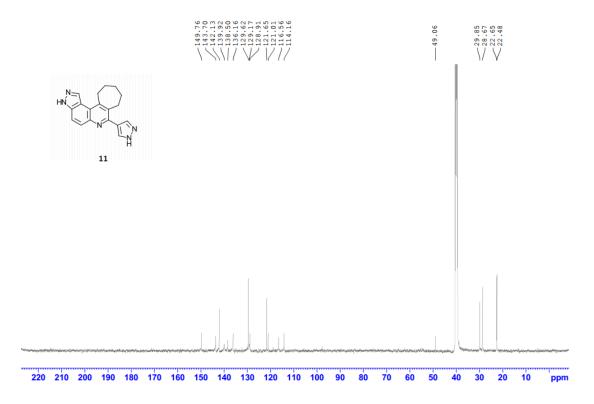


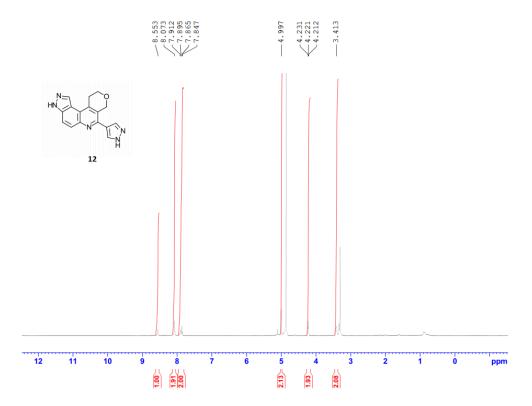
¹³C spectra of 10

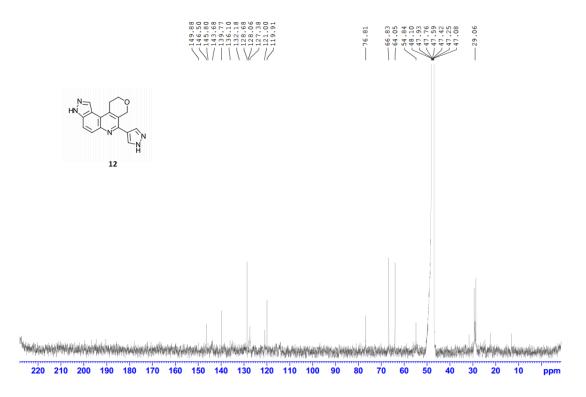


¹H spectra of 11

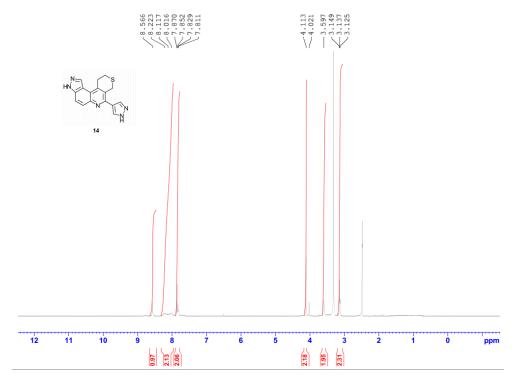




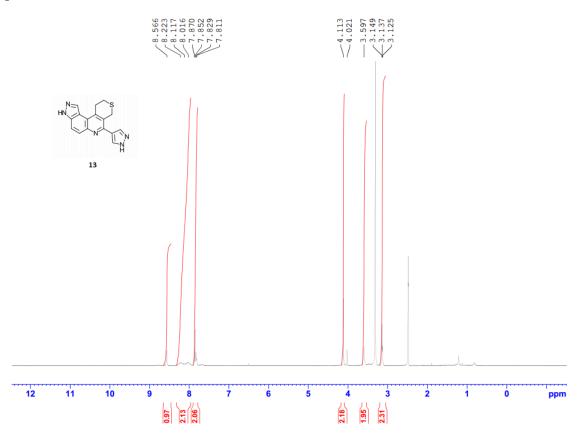




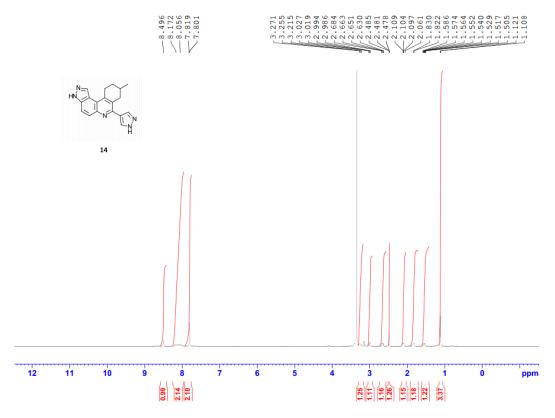
¹H spectra of 13



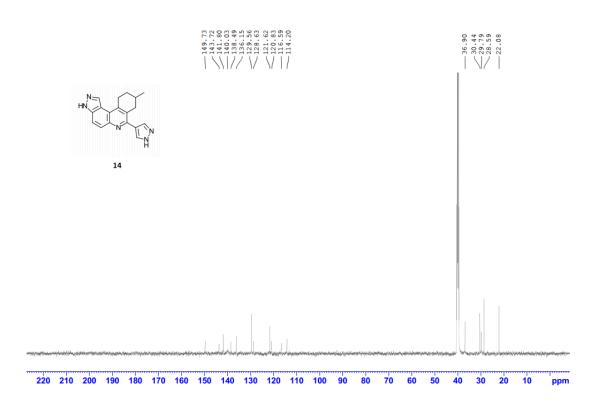
¹³C spectra of 13

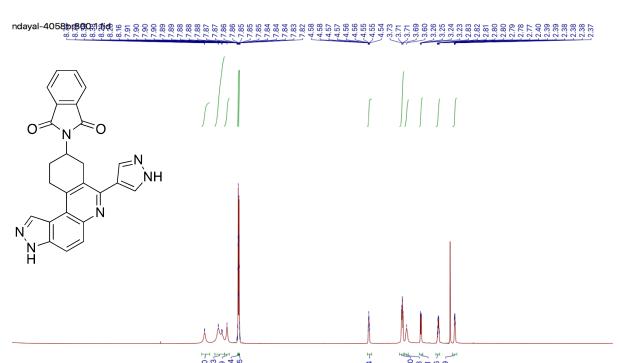


¹H spectra of 14



¹³C spectra of 14





6.5 5.5 f1 (ppm)

4.5

2.5

1.5

0.5

-1.5

-0.5

¹³C spectra of S-1

12.5

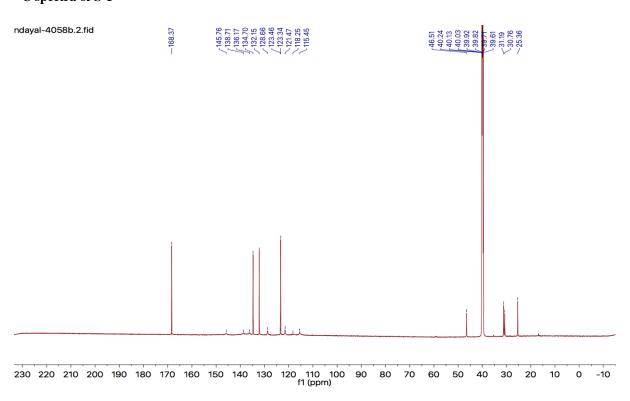
11.5

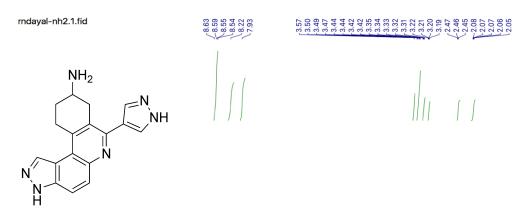
10.5

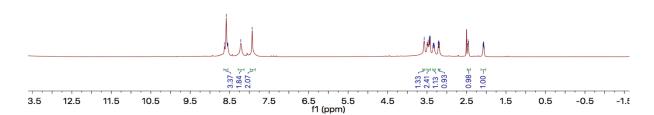
9.5

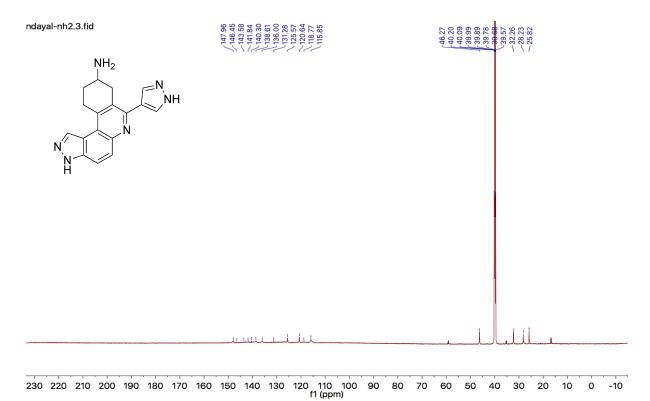
8.5

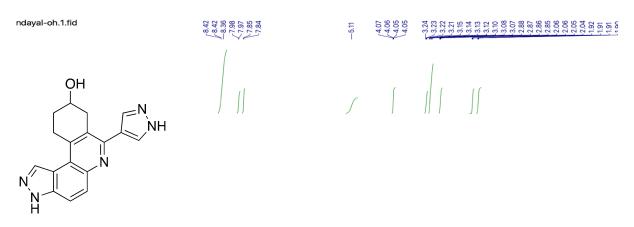
7.5

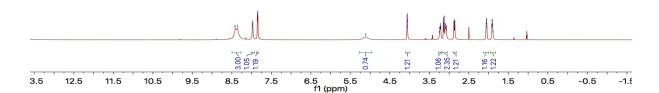




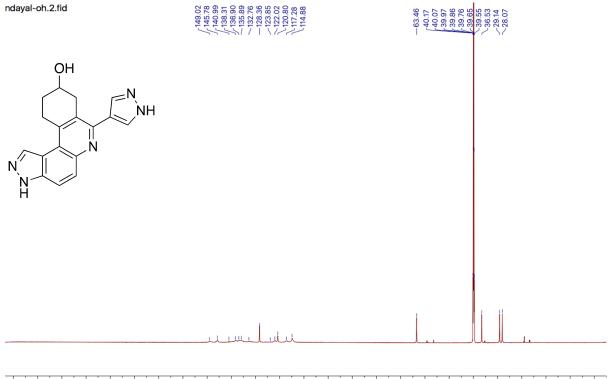




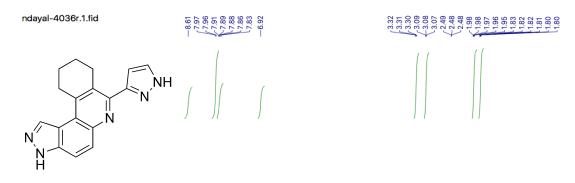


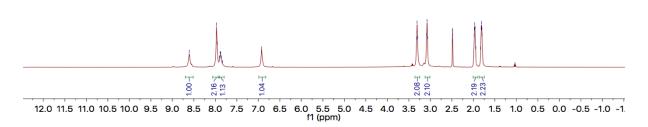


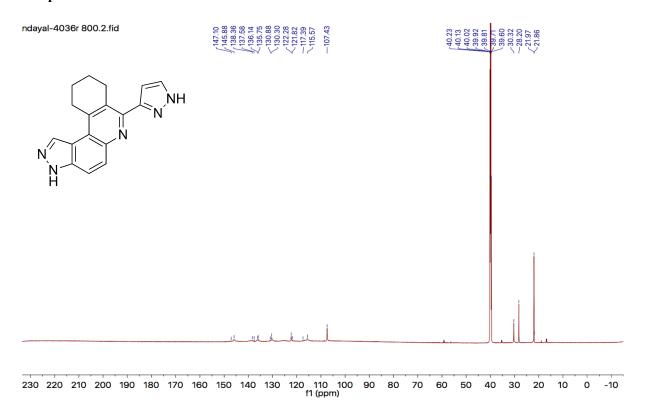
¹³C spectra of 16

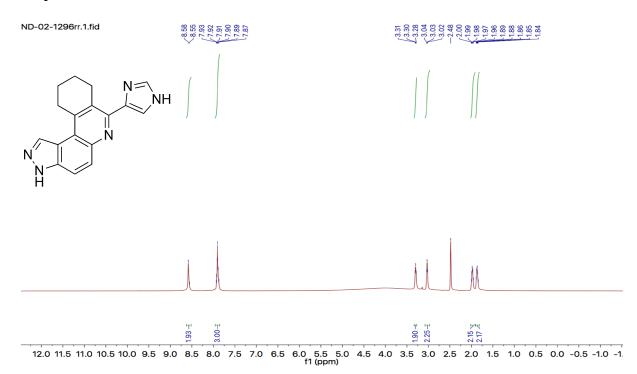


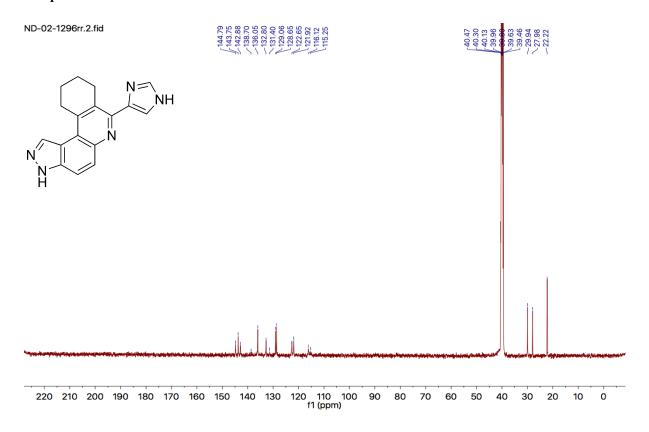
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)

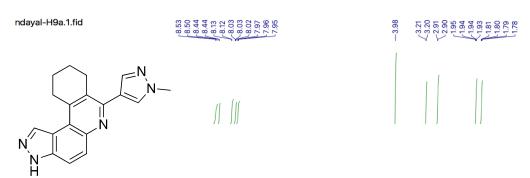


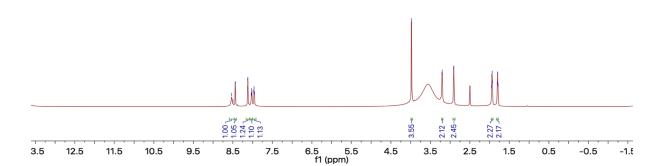


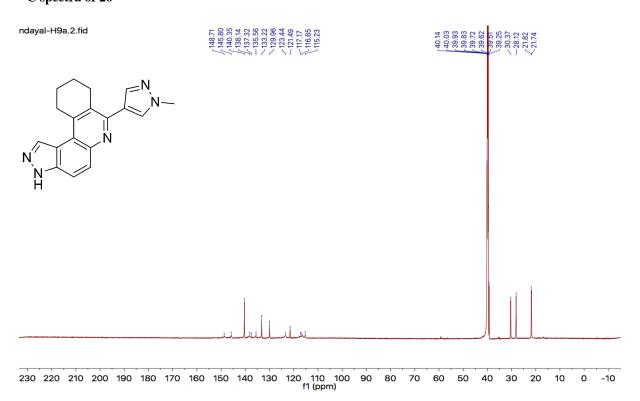






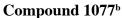






II. HPLC Purity Chromatograms

- a) UV detection wavelength 260 nm, Agilent Eclipse instrument; C18 column (3 μ m, 4.6 × 100 mm²); method: 0 \rightarrow 5 min 50% B, 5 \rightarrow 10 min 50 to 100% B, 10 \rightarrow 24 min 100% B, 24 \rightarrow 25 min 50% B (A: 0.1% NH₄OH in H₂O, B: MeOH), 25 °C.
- b) UV detection wavelength 260 nm, Agilent Eclipse instrument; C18 column (3 μ m, 4.6 × 100 mm²); method: 0 \rightarrow 5 min 50% B, 5 \rightarrow 8 min 50 to 100% B, 8 \rightarrow 24 min 100% B, 24 \rightarrow 25 min 50% B (A: 0.1% NH₄OH in H₂O, B: MeOH), 25 °C.

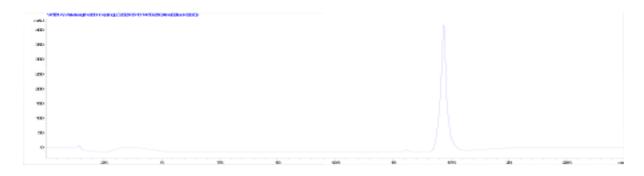




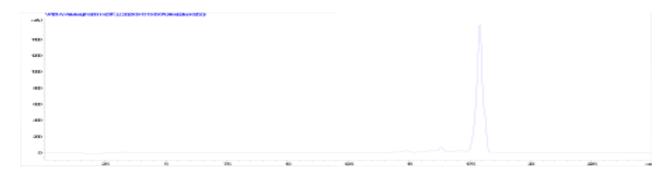
Compound 1a



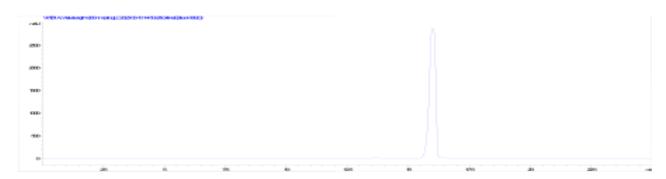
Compound 2^a



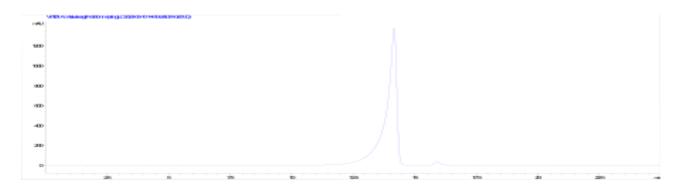
Compound 3^b



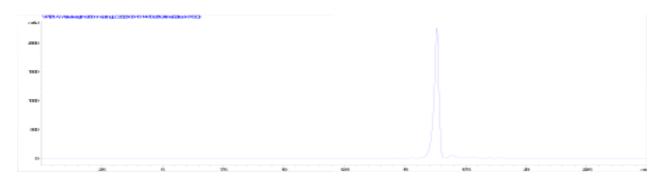
Compound 5^a



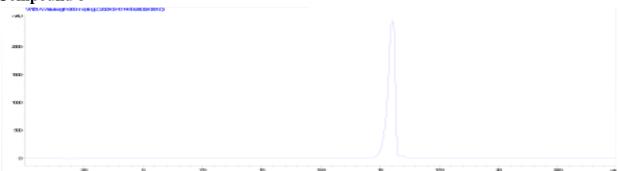
Compound 6^a



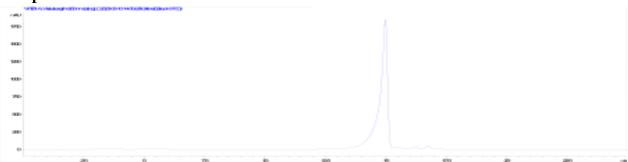
Compound 7^a



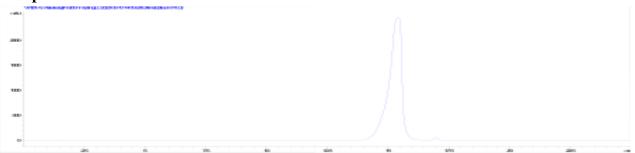
Compound 8^a



Compound 9a



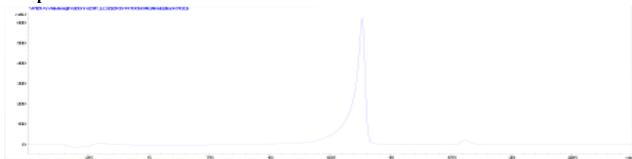
Compound 10^a



Compound 11^b



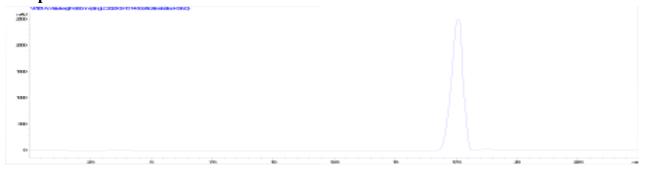
Compound 12^b

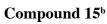


Compound 13^b



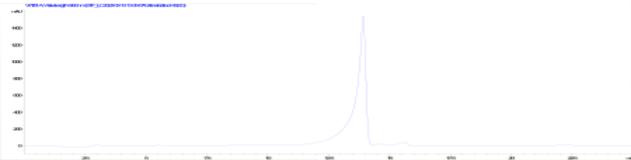
Compound 14^a



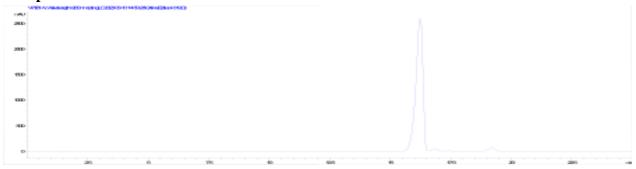




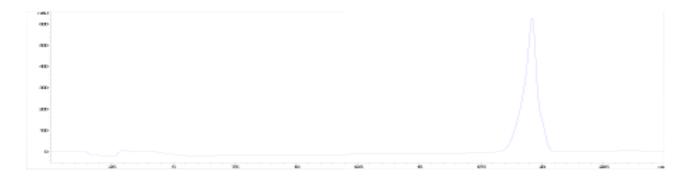
Compound 16^b



Compound 17^a



Compound 21^a



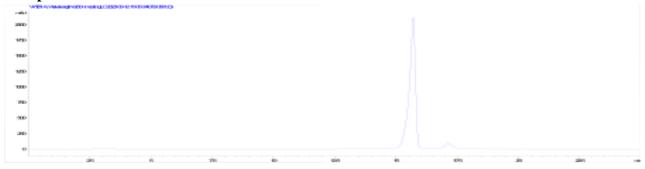
Compound 22^b



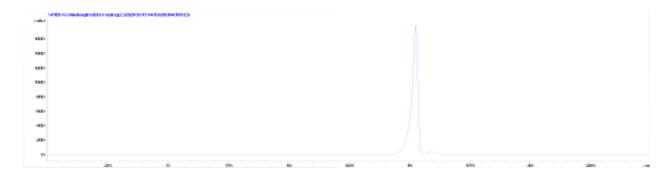
Compound 24^a



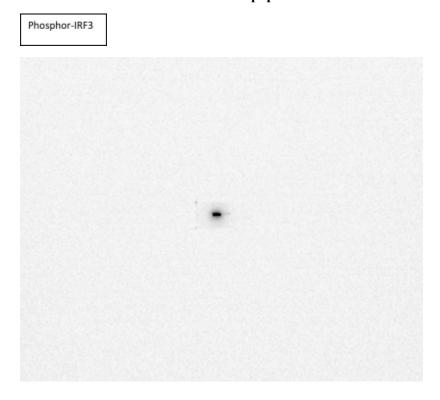
Compound 25^b



Compound 26^a



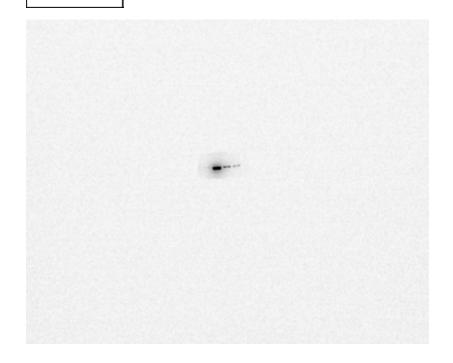
III. Full blots of Western used in the paper



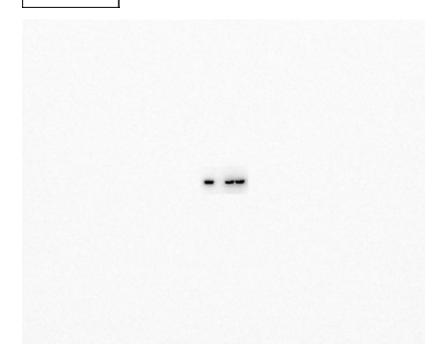
IRF3



Phosphor-STING



STING



Beta-actin

