Azulene-based fluorescent chemosensor for adenosine diphosphate.

Carlos M. López-Alled,[a,b] Sang Jun Park,[c] Dong Joon Lee,[c] Lloyd C. Murfin,[a] Gabriele Kociok-Köhn,[d] Jodie L. Hann,[a] Jannis Wenk,[b,e,*] Tony D. James,[a,b,*] Hwan Myung Kim,[c,*] and Simon E. Lewis,[a,b,*]

a. Department of Chemistry, University of Bath, Bath, BA2 7AY, UK.
b. Centre for Sustainable Circular Technologies, University of Bath, Bath, BA2 7AY, UK. Email: T.D.James@bath.ac.uk, J.H.Wenk@bath.ac.uk, S.E.Lewis@bath.ac.uk
c. Department of Energy Systems Research, Ajou University, Suwon 443-749, South Korea. Email: kimhm@ajou.ac.kr
d. Material and Chemical Characterisation Facility (MC²), University of Bath, Bath, BA2 7AY, UK.
e. Department of Chemical Engineering, University of Bath, Bath, BA2 7AY, UK.

ELECTRONIC SUPPORTING INFORMATION

General Experimental Details . . . . Page S2

UV/Vis absorption spectra . . . . Page S3

Fluorescence data and spectra . . . . Page S7

Synthetic Procedures . . . . Page S14

NMR spectra . . . . Page S20

X-ray crystallographic data . . . . Page S35

References . . . . Page S55

General Experimental Details

Synthetic chemistry and compound characterisation. Azulene was purchased from Alfa Aesar. All other reagents were purchased from Merck. Reactions were carried out under an atmosphere of N_2, through the use of a Schlenk line. Solvent was deoxygenated by channelling a stream of N_2 through the liquid (sparging). Thin layer chromatography (TLC) was carried out on aluminium plates coated with silica gel (Alugram®SIL G/UV 254 nm), and visualisation was achieved by the naked eye (for coloured azulene compounds) and with UV light. Solvents were removed using Büchi rotary evaporators and with high vacuum on a Schlenk line. Flash column chromatography was carried out using Davisil LC 60 Å silica gel (35-70 micron) purchased from Sigma-Aldrich. IR spectra were recorded on a Perkin-Elmer 1600 FT-IR instrument. Capillary melting points were recorded on a Büchi 535 melting point apparatus and are uncorrected. UV-Vis experiments were performed on a Shimadzu UV-1800 UV spectrometer, for which a quartz cuvette of 1 cm path length was used. Fluorescence measurements, unless stated otherwise in the figure caption, were performed on a BMG Labtech CLARIOstar® using Greiner bio-one microplates, 96 well, PS, f-bottom (chimney well), black walled. Data were collected *via* the BMG Labtech Clariostar data analysis software package MARS. All solvents used in fluorescence measurements were HPLC or fluorescence grade and the water was de-ionized. All pH measurements taken during fluorescence/absorption experiments were recorded on a Hanna Instruments HI 9321 Microprocessor pH meter which was routinely calibrated using Fisher Chemicals standard buffer solutions (pH 4.0 - phthalate, 7.0 – phosphate, and 10.0 - borate). HEPES buffer was prepared by generating a 10 mM solution in DMSO/water (1/1, v/v) and adjusting with dilute HCl/NaOH to pH 7.3. ^{1}H and ^{13}C NMR spectra were obtained using a 500 MHz Agilent ProPulse 500 or a 300 MHz Bruker NMR spectrometer, for which proton decoupling was active for ^{13}C NMR. Mass spectrometry was conducted with a microTOF mass spectrometer, with electrospray ionisation (ESI) used as the ionisation method.

Two-photon fluorescence microscopy. Two-photon fluorescence images were acquired with multiphoton microscopes (Leica TCS SP8 MP) and spectral confocal with ×40 objective magnification. **1** was excited at 740 nm by mode-locked femtosecond Ti:Sapphire laser source (Mai Tai HP) with 3.40 W output power, which corresponded to about 1.20×10^6 W cm^{-2} in the focal plane.

Cell culture. All cells were cultured on a glass bottom cell culture dish (NEST) for 2 days with 37 °C, humidity and 5% CO_2 maintained. Before imaging, the medium was changed with serum-free medium and probe (10 µM) was stained. Cell culture medium for HeLa cells (ATCC) was used MEM (WelGene Inc) which was containing 10% FBS (WelGene), penicillin (100 units mL^{-1}) and streptomycin (100 µg mL^{-1}).

Cell viability. To confirm that the probe **1** could not affect viability of cells in our incubation and imaging conditions (200 µM ADP, 50 µM Zn^{2+}, 10 µM Probe **1**), a CCK8 kit was used. 100 µL of HeLa cell suspension was dispensed in a 96-well plate (8000 cells/well). The plates were pre-incubated for 24 h in an incubator (37 °C, 5 % CO_2). Then, various concentration of ADP, Zn^{2+} and probe were added in each well. After addition of substances, further incubation of the plates was conducted for 0.5 h, 3 h and 24 h. Finally 10 µL of CCK8 solution was added to each well and the plates were incubated for 2 h at 37 °C, 5 % CO_2. Using a microplate reader (Varioskan, Thermo Fisher), the absorbance at 450 nm was measured.

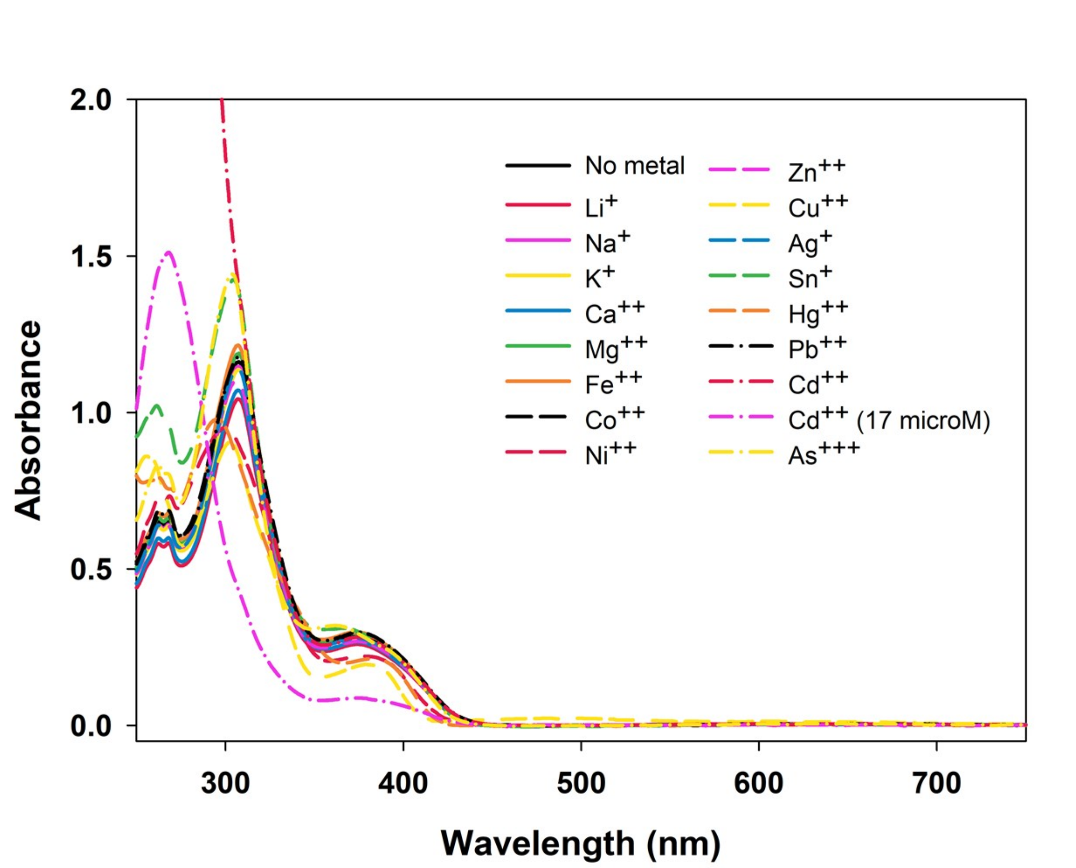


Figure S1: _Top_. Selectivity visual test for **1** (500 µM) in the presence of LiCl (1 mM), NaCl (1 mM), KCl (1 mM), $CaCl_2$ (1 mM), $Mg(NO_3)_2$ (1 mM), $FeSO_4$ (1 mM), $Co(NO_3)_2$ (1 mM), $Ni(acac)_2$ (1 mM), $Zn(NO_3)_2$ (1 mM), $CuCl_2$ (1 mM), $AgNO_3$ (1 mM), $SnCl_2$ (1 mM), $Hg(NO_3)_2$ (1 mM), $Pb(OAc)_2$ (1 mM), $Cd(OAc)_2$ (1 mM) and $As(NO_3)_3$ (1 mM). Spectra were measured after 30 min. The data were obtained in HEPES buffer 50 % H_2O : 50 % MeCN, pH=7.3. _Bottom._ Absorbance spectra of the same solutions diluted ×10.

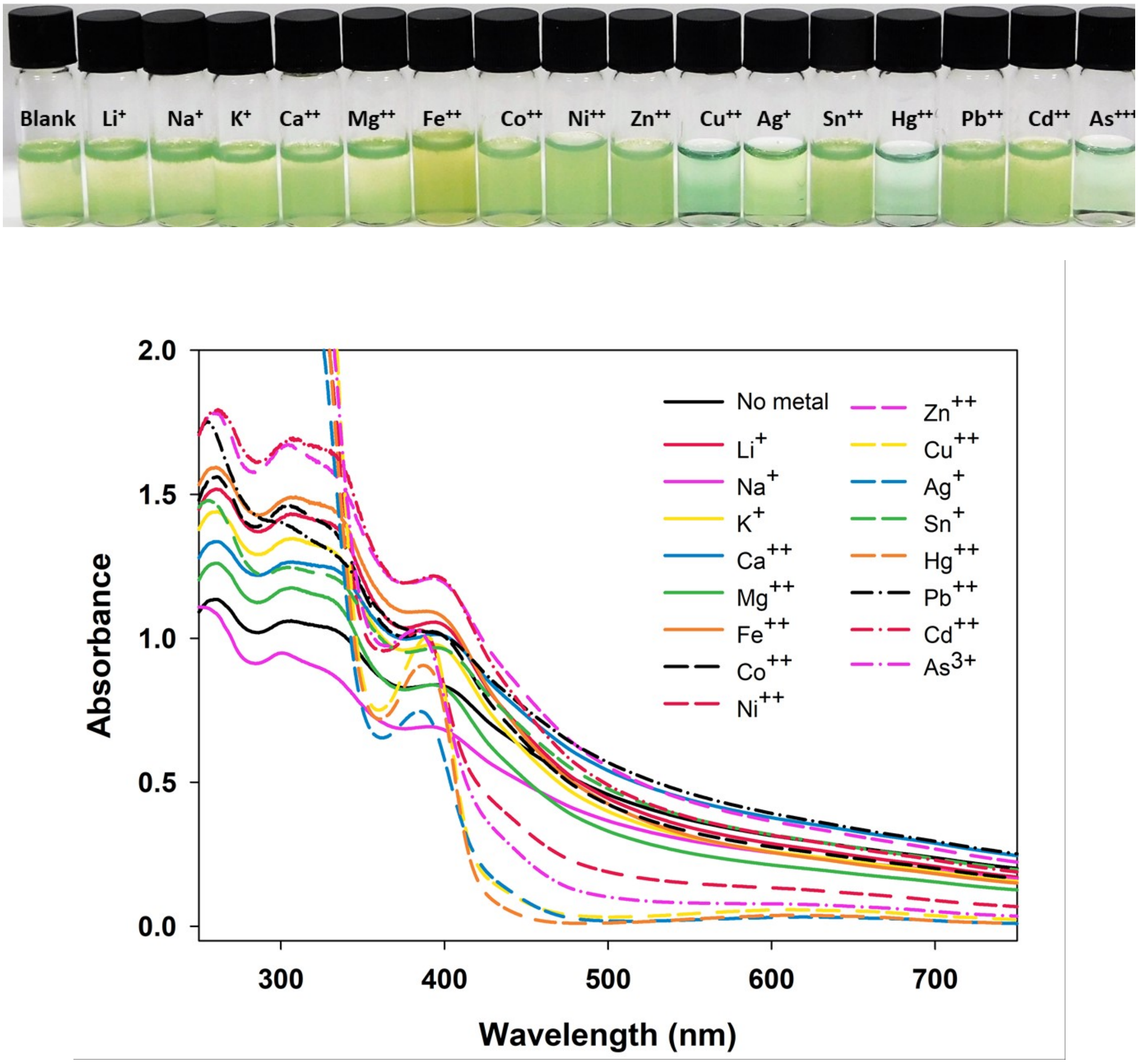
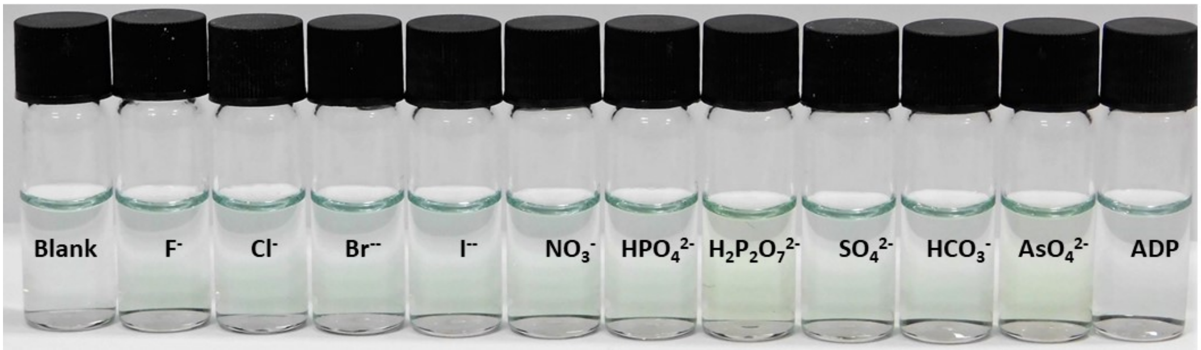


Figure S2: *Top*. Selectivity visual test and absorbance spectra for **2** (500 µM) in the presence of LiCl (1 mM), NaCl (1 mM), KCl (1 mM), $CaCl_2$ (1 mM), $Mg(NO_3)_2$ (1 mM), $FeSO_4$ (1 mM), $Co(NO_3)_2$ (1 mM), $Ni(acac)_2$ (1 mM), $Zn(NO_3)_2$ (1 mM), $CuCl_2$ (1 mM), $AgNO_3$ (1 mM), $SnCl_2$ (1 mM), $Hg(NO_3)_2$ (1 mM), $Pb(OAc)_2$ (1 mM), $Cd(OAc)_2$ (1 mM) and $As(NO_3)_3$ (1 mM). Photos were taken after 30 min. The data were obtained in HEPES buffer 70 % H_2O : 30 % DMSO, pH=7.3. *Bottom*. Absorbance spectra of the same solutions diluted ×10.



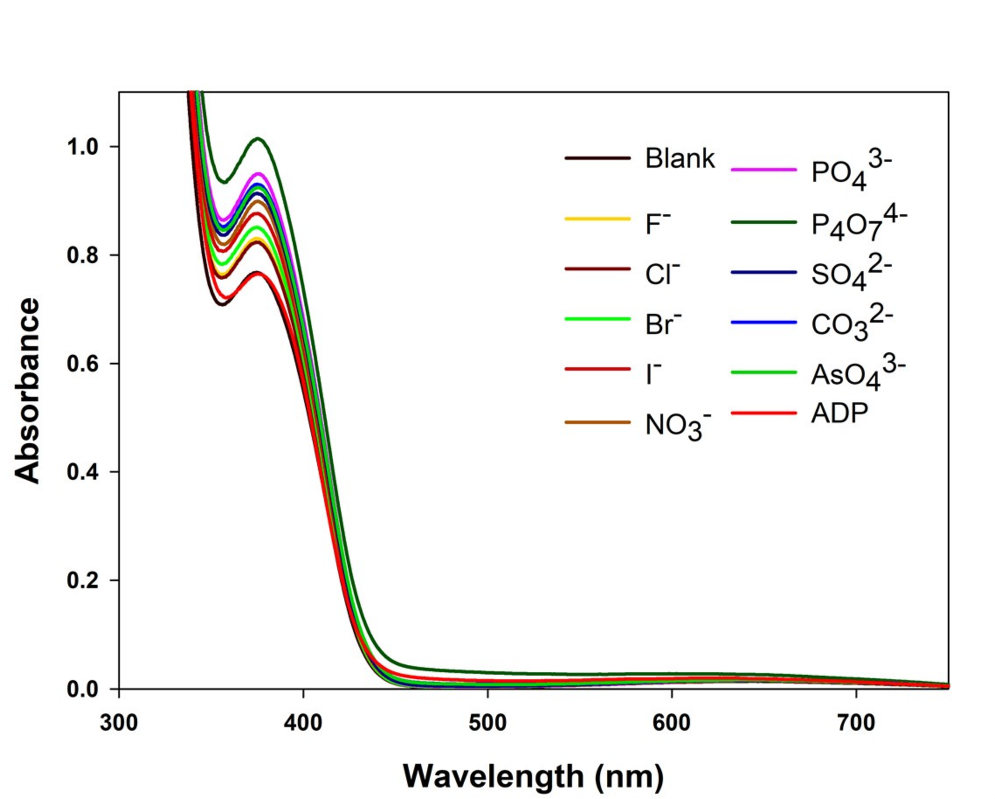


Figure S3: *Top* Selectivity visual test for **1**•2Zn (500 µM) in the presence of NaF (1 mM), NaCl (1 mM), NaBr (1 mM), NaI (1 mM), $NaNO_3$ (1 mM), Na_2HPO_4 (1 mM), $Na_4P_2O_7$ (1 mM), Na_2SO_4 (1 mM), Na_2CO_3 (1 mM), Na_2HAsO_4 (1 mM) and Adenosine 5'-diphosphate sodium salt (1 mM). Photos were measured after 30 min. The data were obtained in HEPES buffer 50 % H_2O : 50 % MeCN, pH=7.3. *Bottom*. Absorbance spectra of the same solutions diluted ×5.

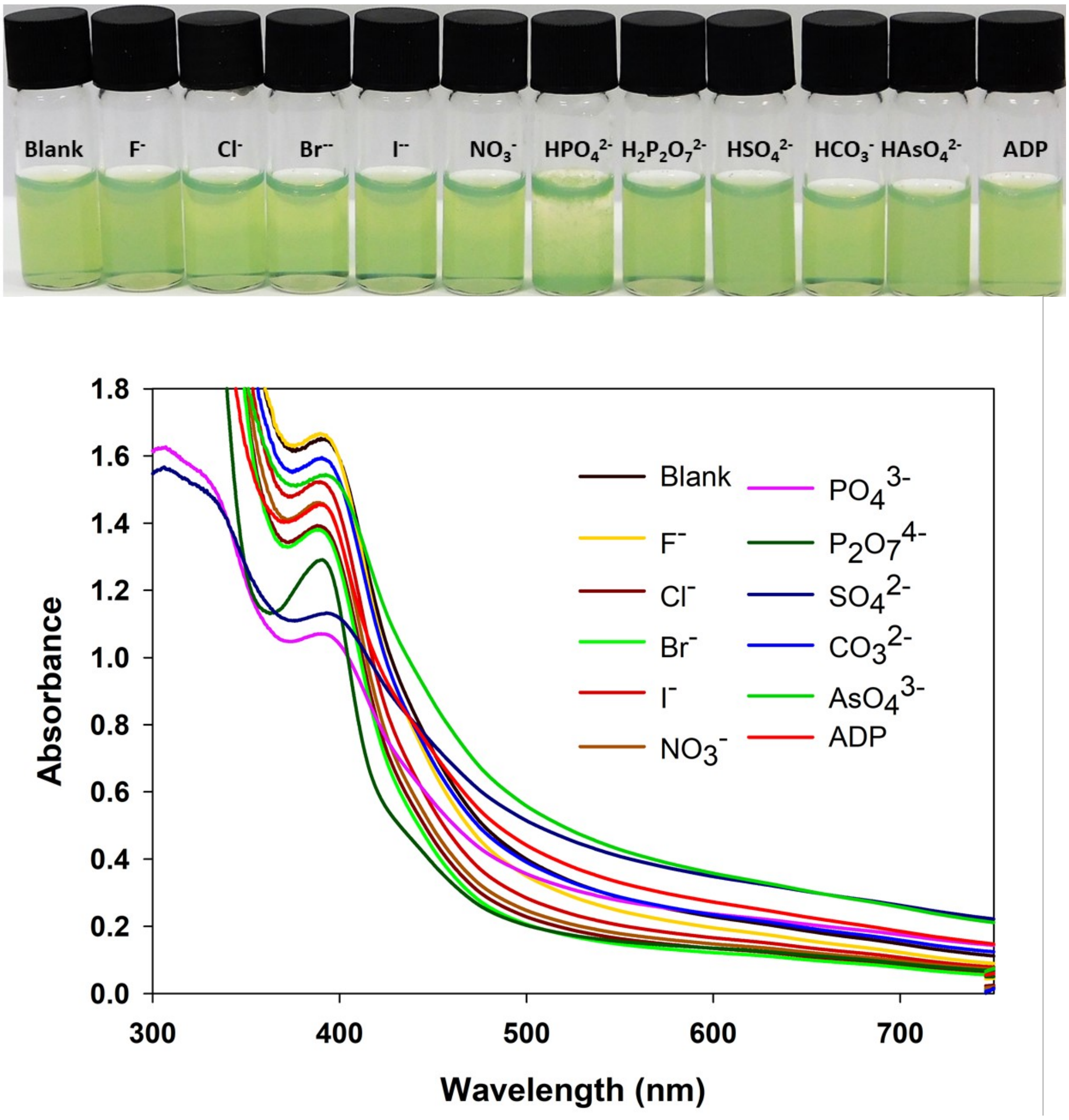


Figure S4: *Top* Selectivity visual test for **2**•2Zn (500 µM) in the presence of NaF (1 mM), NaCl (1 mM), NaBr (1 mM), NaI (1 mM), $NaNO_3$ (1 mM), Na_2HPO_4 (1 mM), $Na_4P_2O_7$ (1 mM), Na_2SO_4 (1 mM), Na_2CO_3 (1 mM), Na_2HAsO_4 (1 mM) and Adenosine 5'-diphosphate sodium salt (1 mM). Photos were measured after 30 min. The data were obtained in HEPES buffer 50 % H_2O : 50 % DMSO, pH=7.3. *Bottom*. Absorbance spectra of the same solutions diluted ×5.

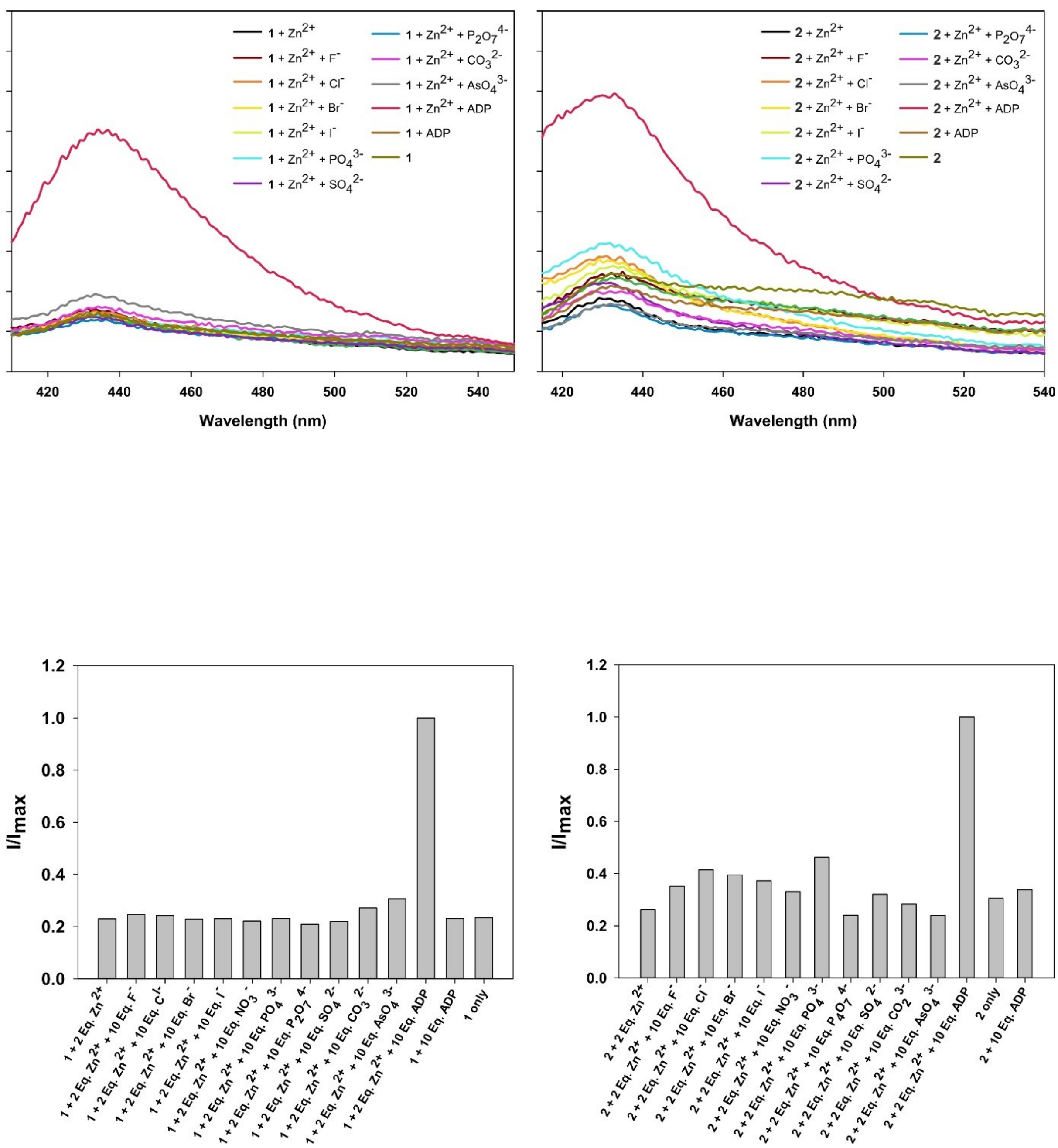


Figure S5: Fluorescence emission spectra for **1**•2Zn (*left*) and **2**•2Zn (*right*), each 100 µM, in the presence of NaF, NaCl, NaBr, NaI, $NaNO_3$, Na_2HPO_4, $Na_4P_2O_7$, Na_2SO_4, Na_2CO_3, Na_2HAsO_4 and ADP sodium salt (all 1 mM). Spectra were measured after 30 min. The data were obtained at 25 °C at λ_{max} = 435 nm. Fluorescence intensities were measured with λ_{exc} = 380 (bandwidth 20) nm on a BMG Labtech CLARIOstar plate reader. For **1**•2Zn, solvent was HEPES buffer 50 % H_2O : 50 % MeCN, pH=7.3; For **2**•2Zn, solvent was HEPES buffer 50 % H_2O : 50 % DMSO, pH=7.3.

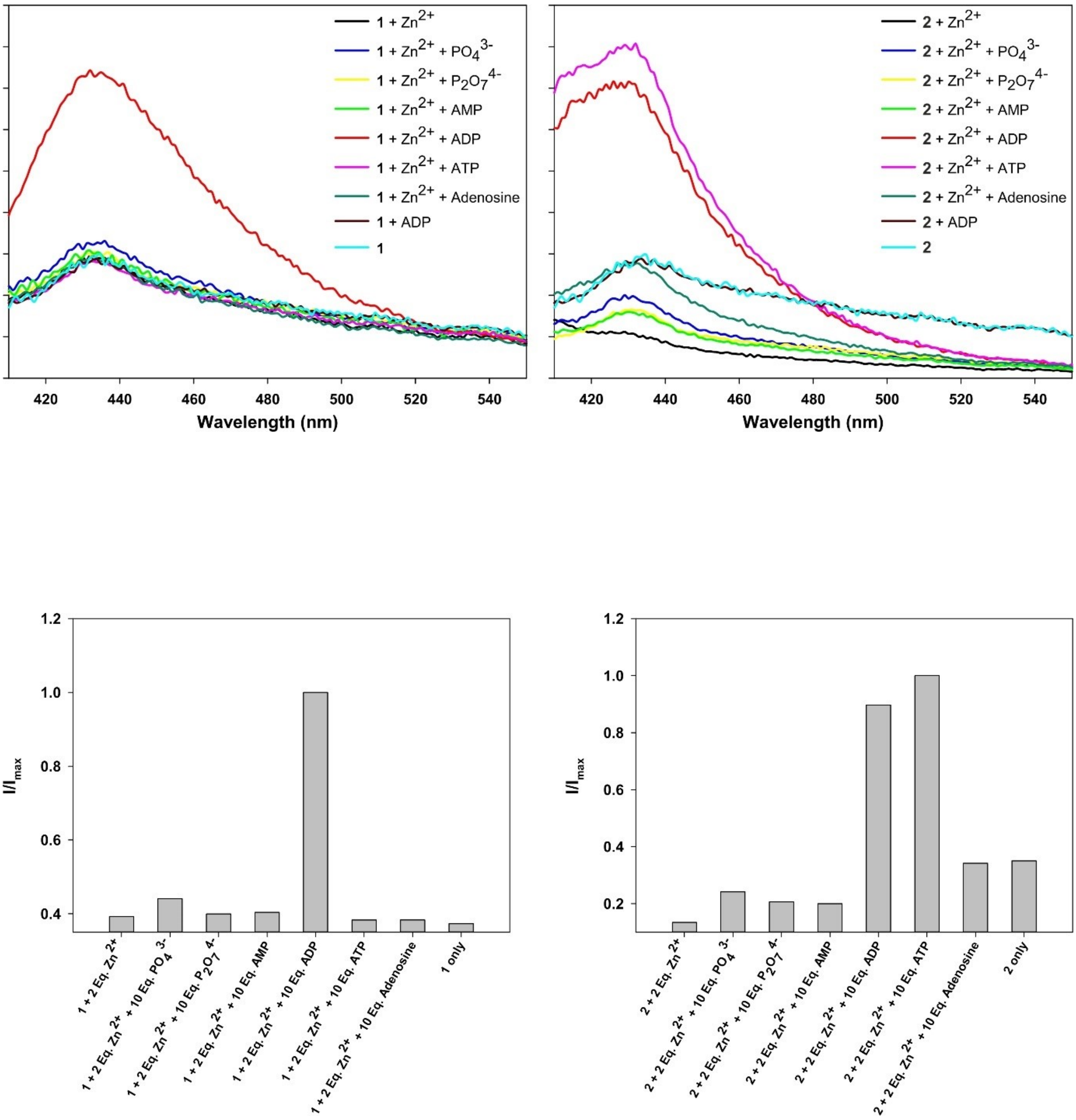


Figure S6: Fluorescence emission spectra for **1**•2Zn (*left*) and **2**•2Zn (*right*), each 100 µM, in the presence of Na_2HPO_4, $Na_4P_2O_7$, AMP sodium salt, ADP sodium salt, ATP sodium salt and adenosine (all 1 mM). Spectra were measured after 30 min. The data were obtained at 25 °C at λ_{max} = 435 nm. Fluorescence intensities were measured with λ_{exc} = 380 (bandwidth 20) nm on a BMG Labtech CLARIOstar plate reader. For **1**•2Zn, solvent was HEPES buffer 50 % H_2O : 50 % MeCN, pH=7.3; For **2**•2Zn, solvent was HEPES buffer 50 % H_2O : 50 % DMSO, pH=7.3.

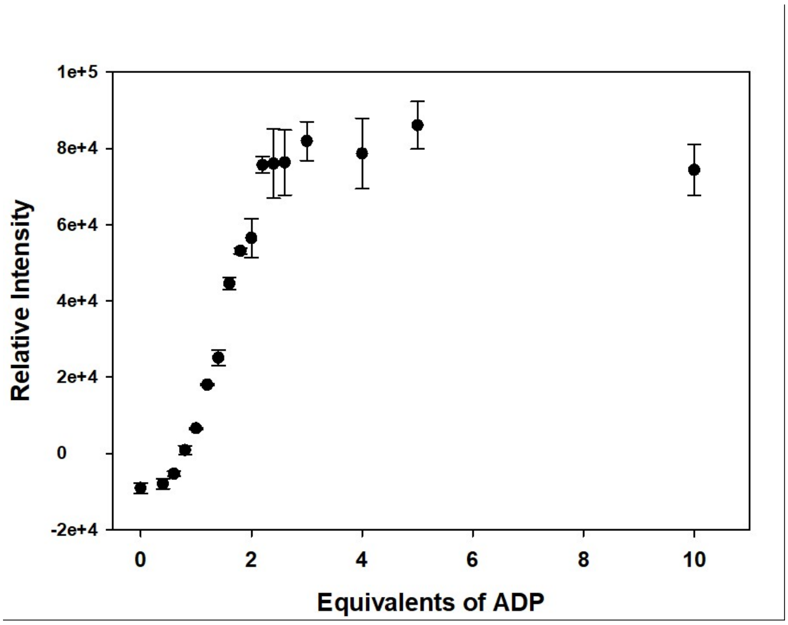


Figure S7: Fluorescence dose-response titration for **1**•2Zn. (100 µM) in the presence of ADP (0, 40, 60, 80, 100, 120, 140, 160, 180, 200, 220, 240, 260, 300, 400, 500, 1000 µM) after 30 min. The data were obtained in HEPES buffer 50 % H_2O : 50 % MeCN, pH=7.3 at 25 °C at λ_{max} = 435 nm. Fluorescence intensities was measured with λ_{exc} = 380 (bandwith 20) nm, on a BMG Labtech CLARIOstar plate reader.

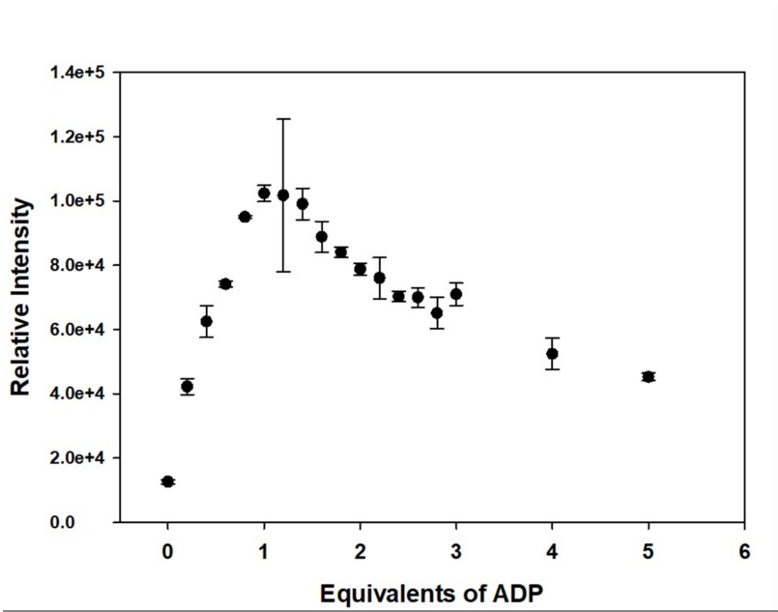


Figure S8: Fluorescence dose-response titration for **2**•2Zn. (100 µM) in the presence of ADP (0, 40, 60, 80, 100, 120, 140, 160, 180, 200, 220, 240, 260, 300, 400, 500 µM) after 30 min. The data were obtained in HEPES buffer 50 % H_2O : 50 % DMSO, pH=7.3 at 25 °C at λ_{max} = 435 nm. Fluorescence intensities was measured with λ_{exc} = 380 (bandwith 20) nm, on a BMG Labtech CLARIOstar plate reader.

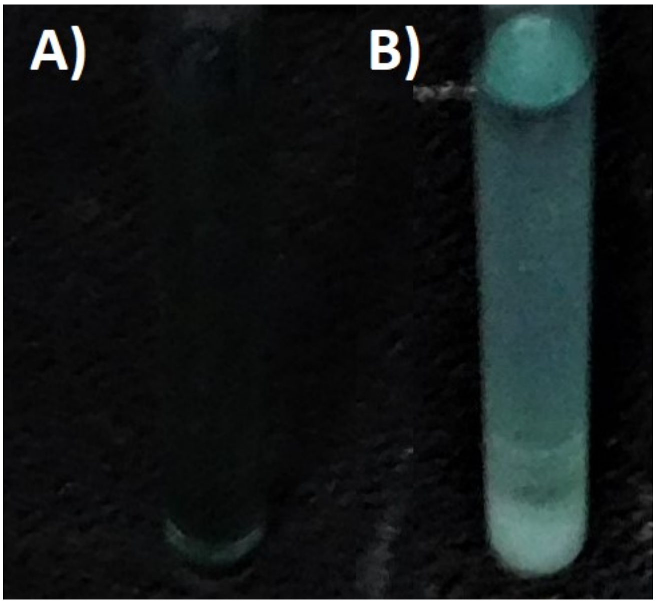
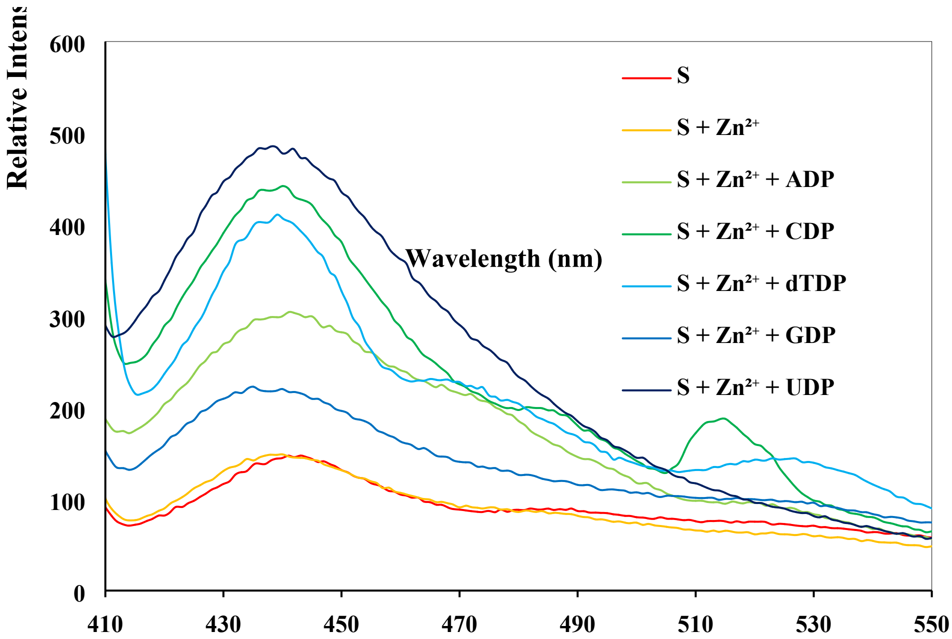


Figure S9: ***A)*** **1**•2Zn (2 mM) in HEPES buffer 50 % H_2O : 50 % MeCN, pH=7.3 at 25 °C. ***B)*** **1**•2Zn (2 mM) in the presence of ADP (4 mM) in HEPES buffer 50 % H_2O : 50 % MeCN, pH=7.3 at 25 °C. Photo taken under 365 nm UV lamp.



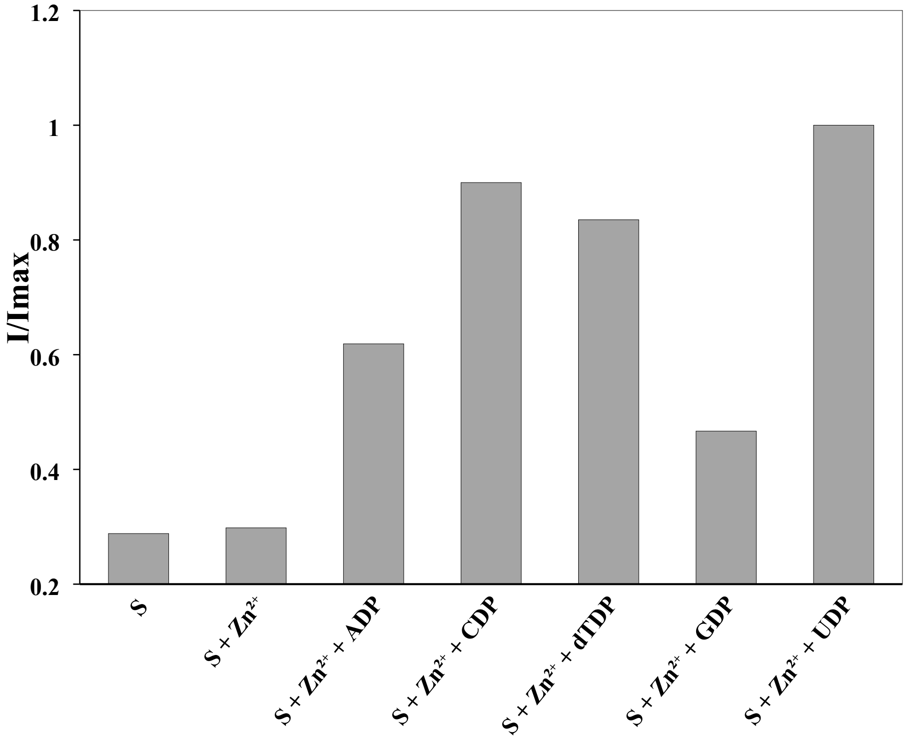


Figure S10: (*top*) Fluorescence emission spectra for **1**•2Zn (100 μM), in the presence of ADP, CDP, dTDP, GDP and UDP (as their respective sodium salts) (all 1 mM). Spectra were measured after 30 min. The data were obtained at 25 °C at λ_{max} = 435 nm in HEPES buffer 50 % H_2O : 50 % MeCN. Fluorescence intensities were measured with λ_{exc} = 380 (bandwidth 20) nm on an Agilent Technologies Cary Eclipse Fluorescence Spectrometer.

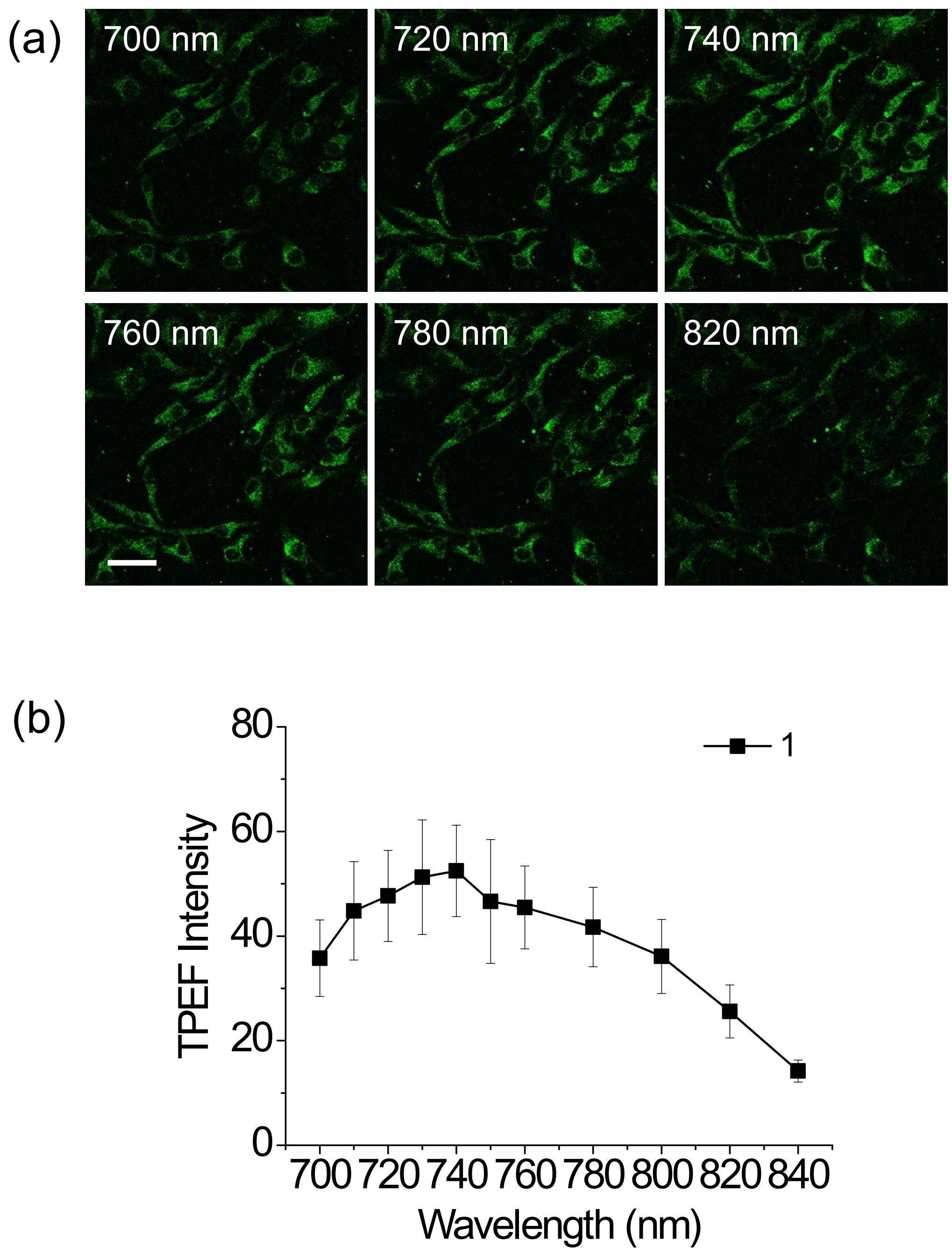


Figure S11: (a) TPM images of HeLa cells, which were stained with **1** (10 μM) for 30 min, at different excitation wavelengths. (b) Average fluorescence intensity of corresponding TPM images. Images were obtained at 400-700 nm detection windows. Scale bar = 50 μm.

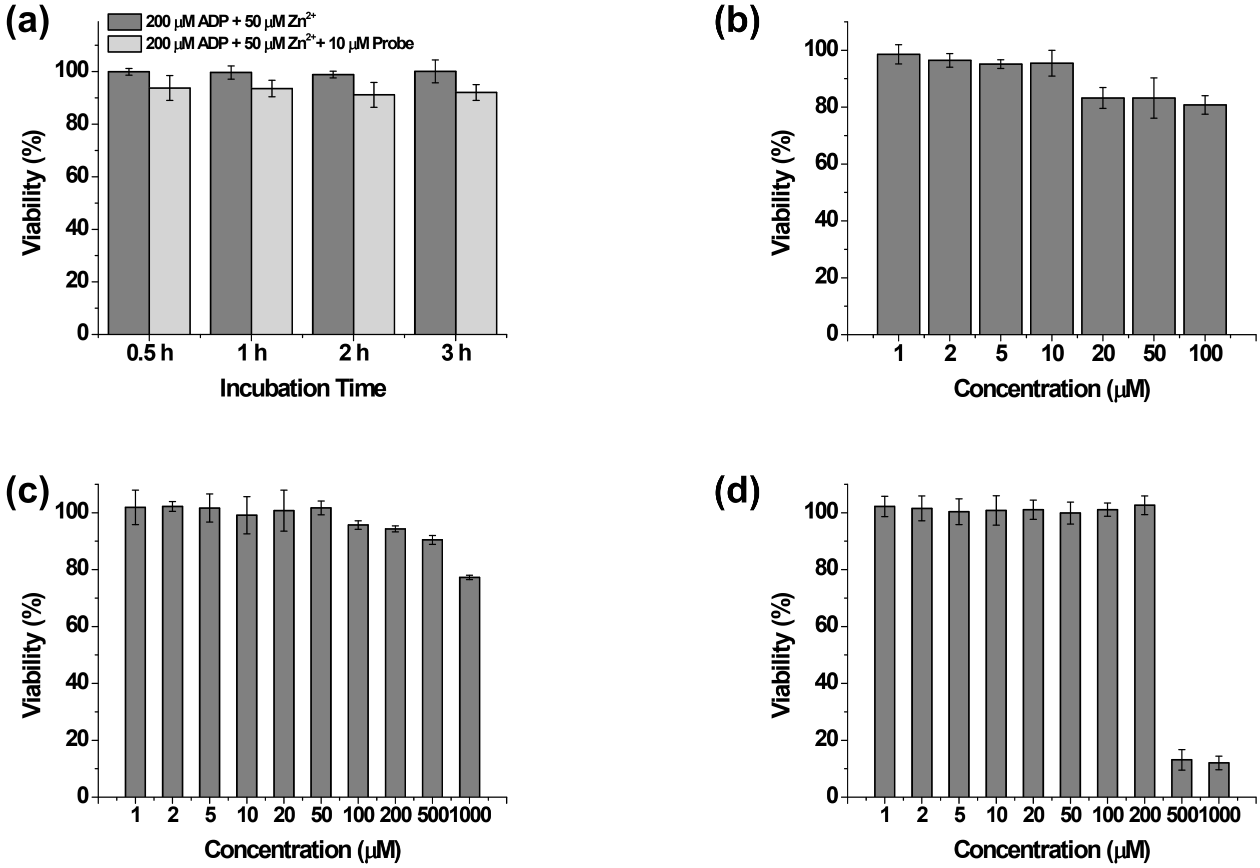
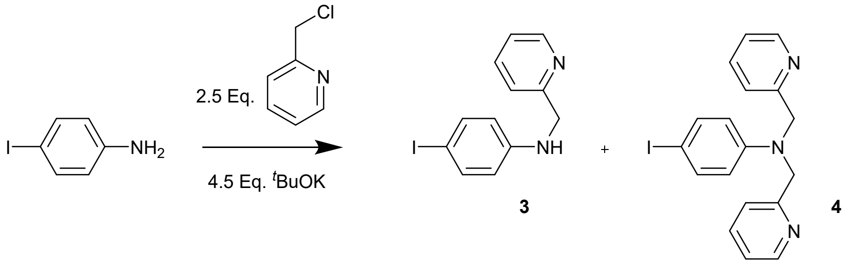


Figure S12: The viability of HeLa cells in the presence of ADP, Zn^{2+} and probe **1**, as measured by using CCK8. (a) The cells were incubated with 200 µM ADP, 50 µM Zn^{2+} or with 200 µM ADP, 50 µM Zn^{2+} and 10 µM probe **1**. The cells were incubated with various concentration of (b) probe **1**, (c) ADP and (d) Zn^{2+} for 24 h. For calculation of viability, the absorbance of CCK8 was measured at 450 nm.

4-Iodo-*N*-2-picolylaniline (**3**) and 4-Iodo-*N*,*N*-bis(2-picolyl)aniline (**4**)

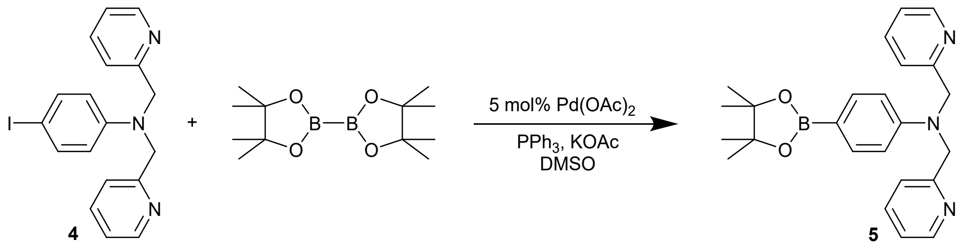


8.00 g of 2-chloromethylpyridine hydrochloride (48.8 mmol, 2.5 eq.) and 4.24 g of 4-iodoaniline (19.4 mmol, 1 Eq.) were poured into a 250 mL round bottom flask containing 80 mL of water. 10.1 grams of potassium *tert*-butoxide (89.2 mmol, 4.6 Eq.) were dissolved in 80 mL of water. This solution was slowly added to the round bottom flask and a colour change from brown to red was observed. The reaction was stirred at room temperature for 4 days. After this, the product was extracted using CH_2Cl_2 (3 × 50 mL), the organic phase was dried with $MgSO_4$ and filtered. Then, the filtrate was concentrated under reduced pressure and the residue was purified by silica column chromatography (CH_2Cl_2/Acetone 3:7 to 1:1) to give **3** as a yellow solid (2.64 g, 8.5 mmol, 44%, R_f = 0.66), followed by **4** as an orange solid (1.77 g, 4.4 mmol, 23%, R_f = 0.50).

3: ^{1}H-NMR (300 MHz, Chloroform-*d*) δ 8.58 (d, *J* = 4.9 Hz, 1H), 7.65 (app td, *J* = 7.7, 1.8 Hz, 1H), 7.42 (d, *J* = 8.8 Hz, 2H), 7.29 (d, *J* = 7.9 Hz, 1H), 7.19 (dd, *J* = 7.3, 5.0 Hz, 1H), 6.45 (d, *J* = 8.8 Hz, 2H), 4.90 (br s, 1H), 4.41 (d, *J* = 4.4 Hz, 2H) ppm. Data in agreement with literature.[1,2]

4: ^{1}H-NMR (300 MHz, Chloroform-*d*) δ 8.58 (d, *J* = 4.9 Hz, 2H), 7.62 (app td, *J* = 7.7, 1.8 Hz, 2H), 7.38 (d, *J* = 8.9 Hz, 2H), 7.22-7.15 (m, 4H), 6.47 (d, *J* = 8.9 Hz, 2H), 4.79 (s, 4H) ppm. Data in agreement with literature.[3,4]

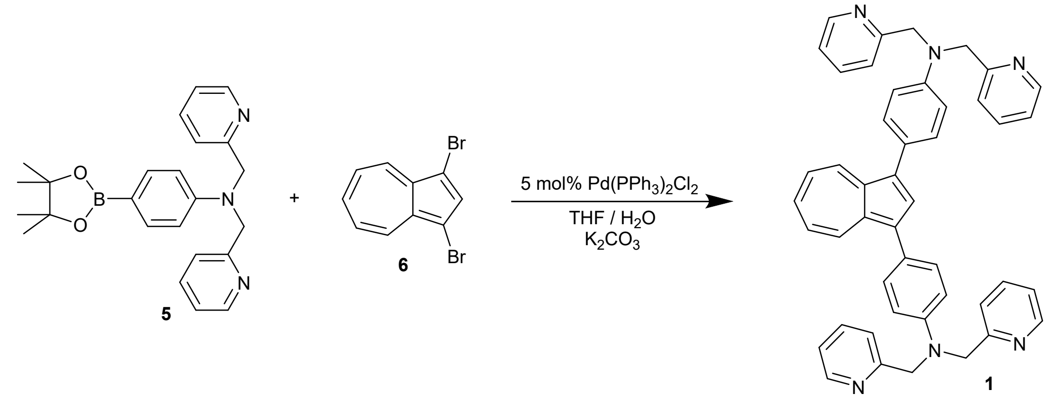
N,*N*-bis(2-Picolyl)-4- (4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (**5**)



1.17 g of **4** (2.76 mmol, 1 Eq.), 31 mg of palladium acetate (0.14 mmol, 0.05 Eq.), 72.4 mg of triphenylphosphine (0.28 mmol. 0.1 Eq.), 745 mg of bis(pinacolato)diboron (3.31 mmol, 1.2 Eq.) and 815 mg of potassium acetate (8.28 mmol, 3 Eq.) were added into a round bottom flask, which was then evacuated and filled with nitrogen. The flask was filled with 20 mL of dry DMSO and the reaction was stirred at 80 °C for 18 h. After this, the reaction mixture was poured into 250 mL of water and the product was extracted using CH_2Cl_2 (3 × 750mL), the organic phase was washed with 50 mL of 5 % $LiCl_{(aq)}$, dried over $MgSO_4$ and filtered. Then, the filtrate was concentrated under reduced pressure and the residue was purified by silica column chromatography (CH_2Cl_2/MeOH 25:1) to give 821 mg of **5** (2.04 mmol, 74 %, R_f = 0.72) as a pale yellow solid.

^{1}H-NMR (300 MHz, Chloroform-*d*) δ 8.58 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 2H), 7.64-7.57 (m, 4H), 7.28-7.13 (m, 4H), 6.69 (d, *J* = 8.8 Hz, 2H), 4.85 (s, 4H), 1.28 (s, 12H) ppm. Data in agreement with literature.[5,6]

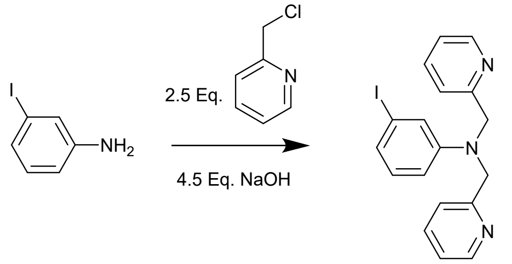
4,4'-(Azulene-1,3-diyl)bis(*N*,*N*-bis(2-picolyl)aniline) (**1**)



81 mg of 1,3-dibromoazulene[7] (**6**, 0.28 mmol, 1 Eq.), 454 mg of **5** (1.13 mmol, 4 Eq.), 10 mg of $Pd(PPh_3)Cl_2$ (0.014, 0.05 Eq.) and 156 mg of potassium carbonate (1.13 mmol, 4 Eq.) were added to a 50 mL round bottom flask, this was evacuated and filled with nitrogen, then filled with 20 mL of a THF/water (4:1) mixture that had been previously degassed by freeze-pump-thaw. The mixture was allowed to react for 18 hours at 75 °C. The product was extracted using CH_2Cl_2 (3 × 50 mL), the organic phase was dried over $MgSO_4$ and filtered. The filtrate was concentrated under reduced pressure and the residue was purified by silica column chromatography (CH_2Cl_2/MeOH 25:1), followed by recrystallisation from acetonitrile to give 121 mg of **1** (0.17 mmol, 63%, R_f = 0.50) as a green solid (blue in CH_2Cl_2 solution).

1: ^{1}H-NMR (500 MHz, DMSO-*d*$_6$) δ 8.58 (d, *J* = 4.9 Hz, 4H), 8.28 (d, *J* = 9.7 Hz, 2H), 7.91 (s, 1H), 7.76 (app td, *J* = 7.7, 1.9 Hz, 4H), 7.49 (t, *J* = 9.8 Hz, 1H), 7.37 (d, *J* = 7.9 Hz, 4H), 7.34 (d, *J* = 8.4 Hz, 4H), 7.28 (dd, *J* = 7.5, 4.9 Hz, 4H), 6.98 (app t, *J* = 9.8 Hz, 2H), 6.77 (d, *J* = 8.5 Hz, 4H), 4.90 (s, 8H) ppm. ^{13}C-NMR (126 MHz, acetone-*d*$_6$) δ 160.30, 150.43, 148.08, 139.63, 137.42, 137.05, 136.71, 136.57, 131.45, 131.12, 126.47, 123.16, 122.87, 121.96, 113.73, 58.33 ppm. IR *v*: 3051, 3006, 2926, 2858, 1737, 1610, 1589, 1567, 1531, 1500, 1470, 1433, 1380, 1346, 1296, 1271, 1231, 1199, 1178, 1119, 1093, 1044, 1011, 993, 967, 947, 888, 862, 815, 753, 738, 722, 694, 670, 657 cm^{-1}. Melting point = 94 ± 2 °C. HRMS (ESI+) calcd for $[C_{46}H_{38}N_6+H]^+$ 675.3231; found 675.3205. Calcd for $[C_{46}H_{38}N_6+Na]^+$ 697.3050; found 697.3029.

3-Iodo-*N*,*N*-bis(2-picolyl)aniline (**7**)

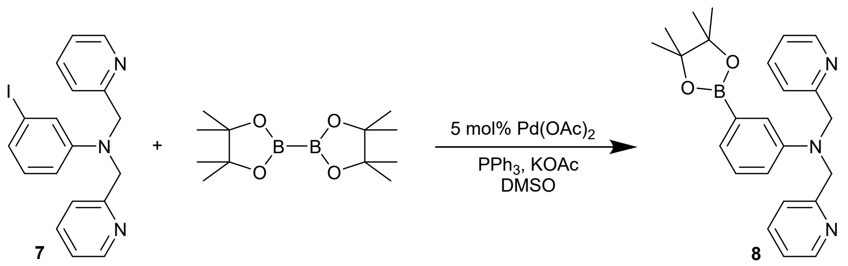


7

9.25 g of 2-chloromethylpyridine hydrochloride (56.4 mmol, 2.5 Eq.) and 2.71 mL of 3-Iodoaniline (22.6 mmol, 1.0 Eq.) were poured in a 250 mL round bottom flask containing 80 mL of water. 4.06 g of sodium hydroxide (101.5 mmol, 4.5 Eq.) were dissolved in 80 mL of water, then this solution was slowly added to the round bottom flask and a colour change from brown to red was observed. The reaction was stirred at room temperature for 4 days. After this, the product was extracted using CH_2Cl_2 (3 × 50 mL), the organic phase was dried over $MgSO_4$ and filtered. Then, the filtrate was concentrated under reduced pressure and the residue was purified by silica column chromatography (CH_2Cl_2/Acetone 3:7 to 1:1) to give 1.00 g of **7** (2.5 mmol, 11%, R_f = 0.50) as a an orange oil.

^{1}H-NMR (500 MHz, Chloroform-*d*) δ 8.59 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 2H), 7.63 (app td, *J* = 7.7, 1.8 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 7.17 (ddd, *J* = 7.6, 4.8, 1.1 Hz, 2H), 7.07 (dd, *J* = 2.6, 1.5 Hz, 1H), 7.03 (d, *J* = 7.7 Hz, 1H), 6.84 (dd, *J* = 8.5, 7.7 Hz, 1H), 6.64 (ddd, *J* = 8.5, 2.7, 0.9 Hz, 1H), 4.77 (s, 4H) ppm. ^{13}C-NMR (126 MHz, Chloroform-*d*) δ 158.19, 149.95, 149.64, 137.00, 130.76, 126.37, 122.32, 121.32, 120.87, 111.97, 95.71, 57.15 ppm. IR *v*: 2988, 2971, 2901, 1583, 1510, 1488, 1470, 1430, 1381, 1341, 1277, 1253, 1224, 1174, 1088, 1043, 978, 964, 941, 794, 751, 731, 682 cm^{-1}. HRMS (ESI+) calcd for $[C_{18}H_{16}IN_3+H]^+$ 402.0462; found 402.0474.

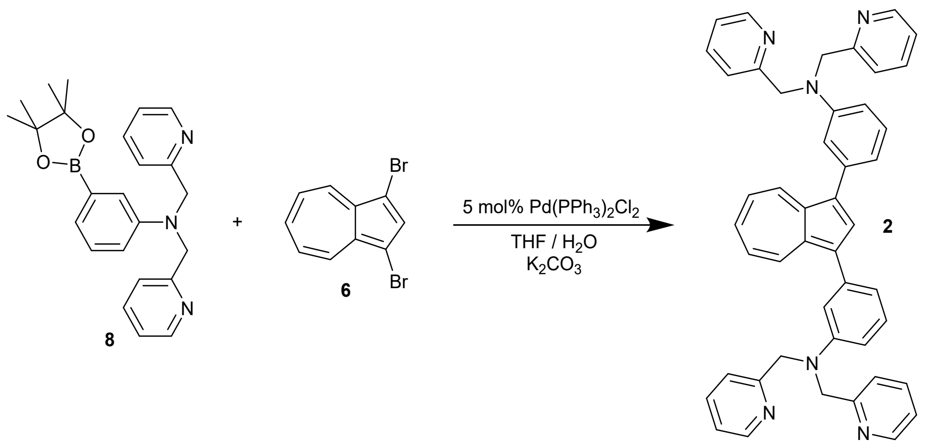
N,N-Bis(2-picolyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) aniline (**8**)



1.00 g of **7** (2.5 mmol, 1 Eq.), 28 mg of palladium acetate (0.12 mmol, 0.05 Eq.), 65.3 mg of triphenylphosphine (0.25 mmol, 0.1 Eq.), 762 mg of bis(pinacolato)diboron (3 mmol, 1.2 Eq.) and 733 mg of potassium acetate (7.47 mmol, 3 Eq.) were added to a round bottom flask. This was evacuated and filled with nitrogen. The flask was filled with 20 mL of dry DMSO and the reaction was stirred at 80 °C for 18 hours. After this, the reaction mixture was poured into 150 mL of water and the product was extracted using CH_2Cl_2 (3 × 50 mL). The organic phase was washed with 50 mL of 5% $LiCl_{(aq)}$, dried over $MgSO_4$ and filtered. Then, the filtrate was concentrated under reduced pressure and the residue was purified by silica column chromatography (CH_2Cl_2/MeOH 25:1) to give 768 mg of **8** (1.92 mmol, 77%, R_f = 0.65) as an orange oil.

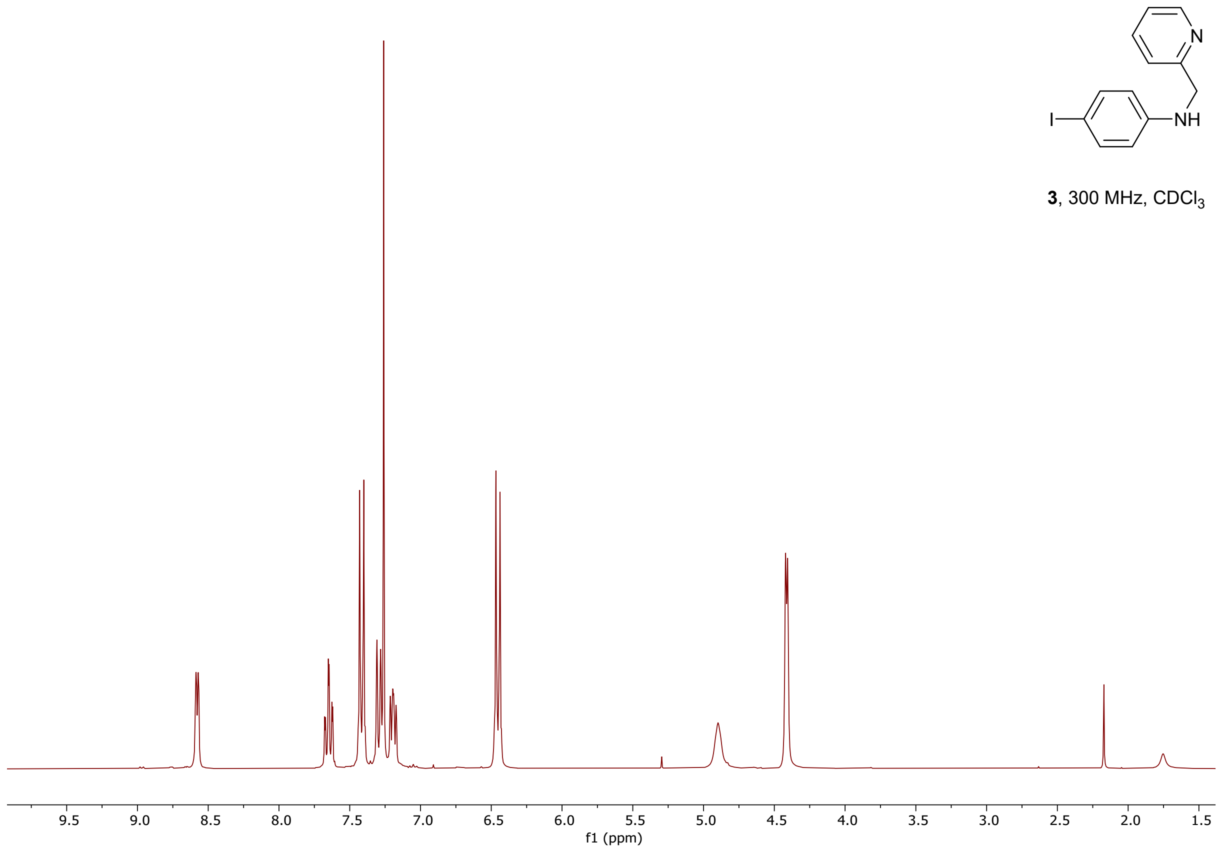
^{1}H-NMR (500 MHz, Chloroform-*d*) δ 8.57 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 2H), 7.59 (app td, *J* = 7.7, 1.8 Hz, 2H), 7.27-7.23 (m, 3H), 7.19-7.12 (m, 4H), 6.78 (app dt, *J* = 7.3, 2.6 Hz, 1H), 4.82 (s, 4H), 1.28 (s, 12H) ppm. ^{13}C-NMR (126 MHz, Chloroform-*d*) δ 159.01, 149.72, 147.85, 136.86, 128.87, 123.92, 122.07, 121.08, 118.51, 115.69, 83.73, 56.90, 24.93 ppm. One carbon environment was not observed (C adjacent to B). IR *v*: 3082, 2976, 2925, 2854, 1605, 1548, 1529, 1507, 1469, 1434, 1390, 1352, 1277, 1231, 1200, 1140, 1098, 1046, 1008, 991, 963, 942, 907, 887, 860, 810, 769, 750, 695, 670, 652 cm^{-1}. HRMS (ESI+) calcd for $[C_{24}H_{28}BN_3O_2+H]^+$ 402.2347; found 402.2351.

3,3'-(Azulene-1,3-diyl)bis(*N*,*N*-bis(2-picolyl)aniline) (2)

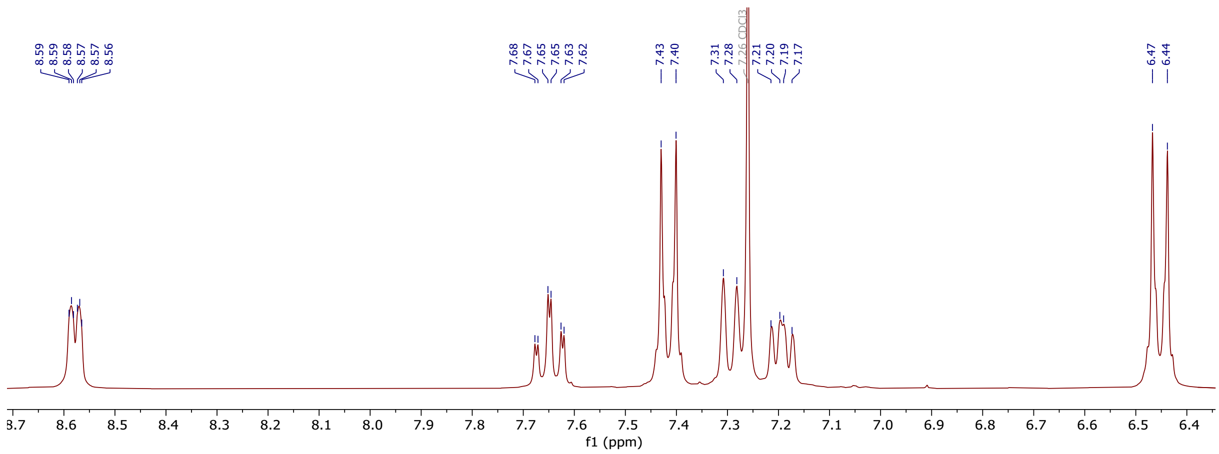


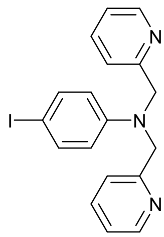
138 mg of 1,3-dibromoazulene[7] (**6**, 0.47 mmol, 1 Eq.), 750 mg of **8** (1.87 mmol, 4 Eq.), 16 mg of $Pd(PPh_3)Cl_2$ (0.02 mmol, 0.05 Eq.) and 259 mg of potassium carbonate (1.87 mmol, 4 Eq.) were added to a 50 mL round bottom flask, this was evacuated and filled with nitrogen, then filled with 20 mL of a THF/water (4:1) mixture that had been previously degassed by freeze-pump-thaw. The mixture was allowed to react for 18 hours at 75 °C. The product was extracted using CH_2Cl_2 (3 × 50 mL), the organic phase was dried over $MgSO_4$ and filtered. Then, the filtrate was concentrated under reduced pressure and the residue was purified by silica column chromatography (CH_2Cl_2/MeOH 25:1), followed by recrystallisation from acetonitrile to give 276 mg of **2** (0.41 mmol, 87%, R_f = 0.50) as a green solid (blue in CH_2Cl_2 solution).

^{1}H-NMR (500 MHz, Acetone-d_6) δ 8.57 (s, 4H), 8.19 (d, *J* = 7.1 Hz, 2H), 7.88 (s, 1H), 7.76 (app t, *J* = 7.6 Hz, 4H), 7.53 (t, *J* = 9.8 Hz, 1H), 7.44 (d, *J* = 7.9 Hz, 4H), 7.30-7.21 (m, 6H), 6.98-6.85 (m, 6H), 6.74 (d, *J* = 7.9 Hz, 2H), 4.96 (s, 8H) ppm. ^{13}C-NMR (126 MHz, Methanol-d_4) δ 160.43, 150.21, 149.11, 139.69, 139.18, 138.96, 137.83, 137.61, 136.72, 132.01, 130.61, 124.34, 123.75, 122.93, 120.11, 115.53, 112.31, 58.43 ppm. IR *v*: 3048, 3005, 2958, 2925.5, 2872, 2160, 1979, 1728, 1589, 1569, 1491, 1470, 1433, 1383, 1342, 1274, 1249, 1226, 1194, 1176, 1146, 1091, 1047, 993, 968, 946, 856, 776, 753, 703, 654 cm^{-1}. Melting point = 90±4 °C. HRMS (ESI+) calcd for $[C_{46}H_{38}N_6+H]^+$ 675.3231; found 675.3377.

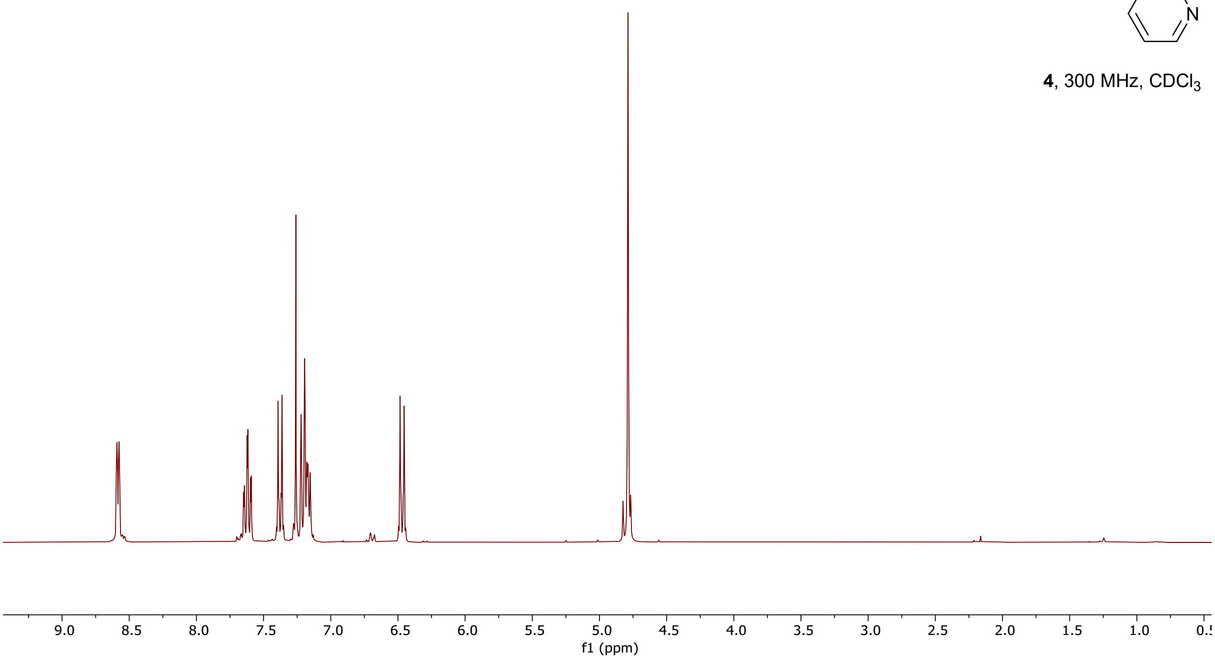


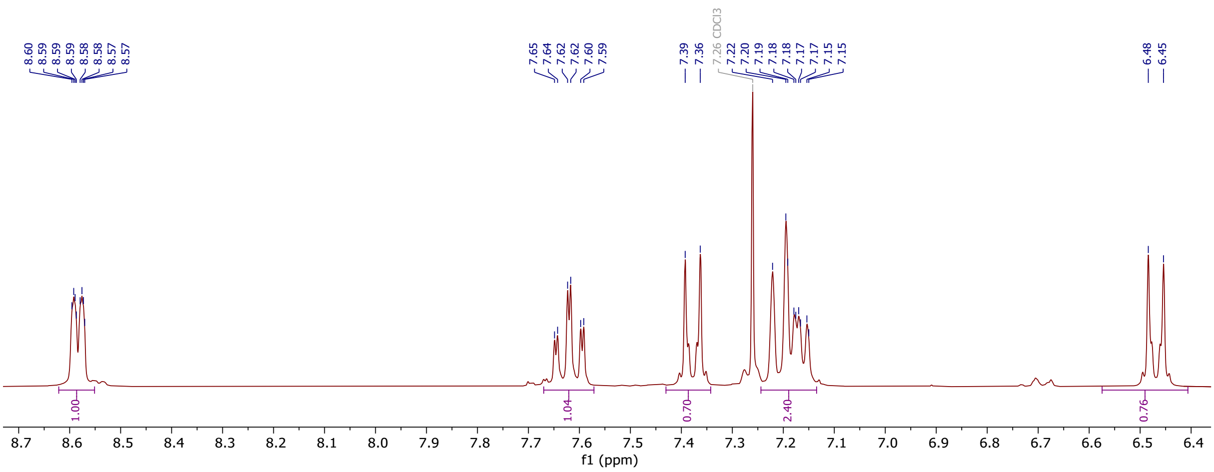
3, 300 MHz, $CDCl_3$

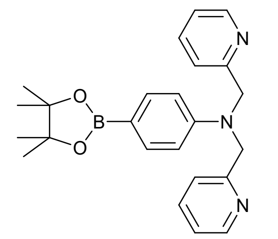




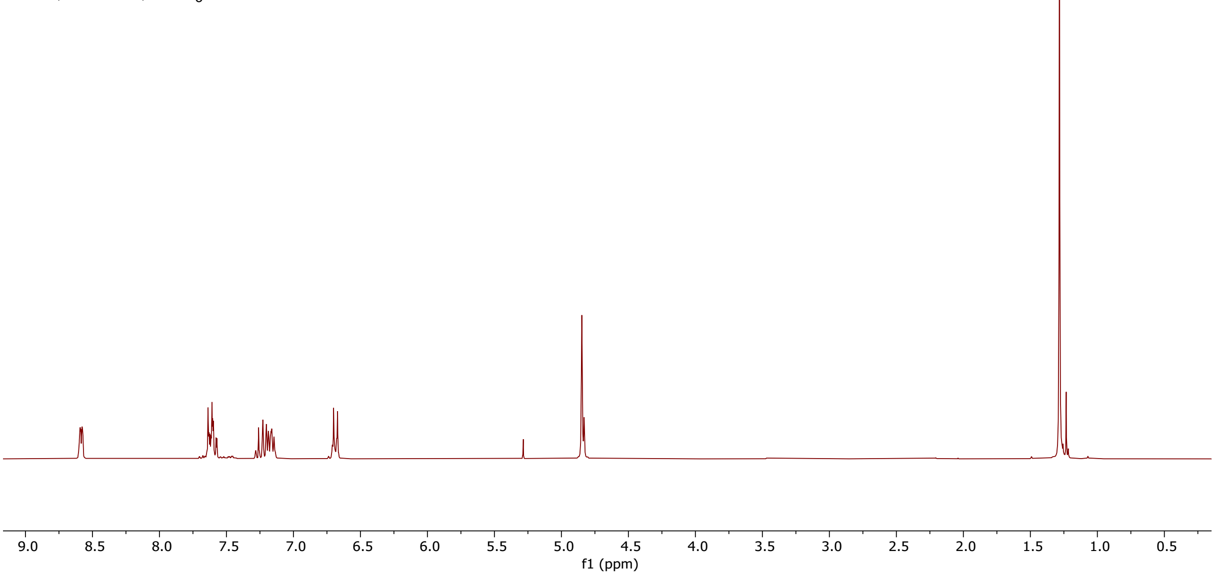
4, 300 MHz, $CDCl_3$

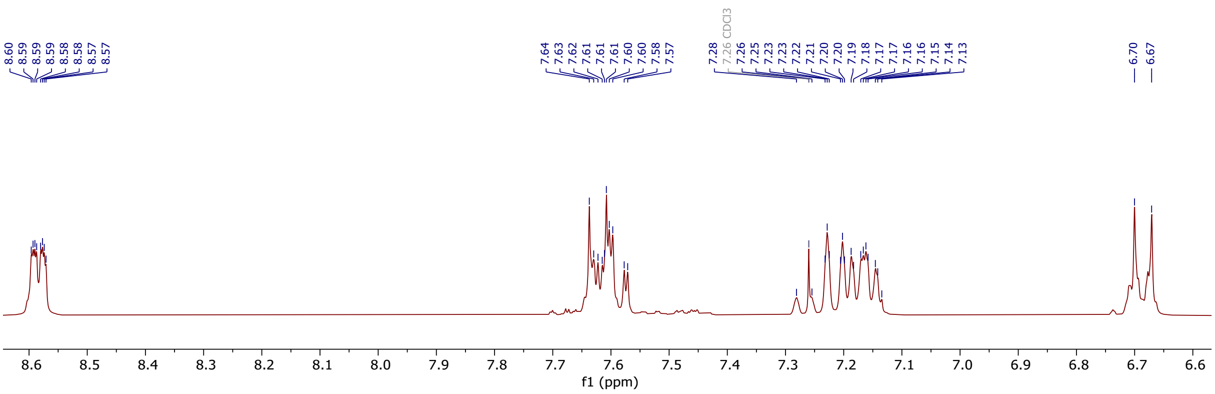


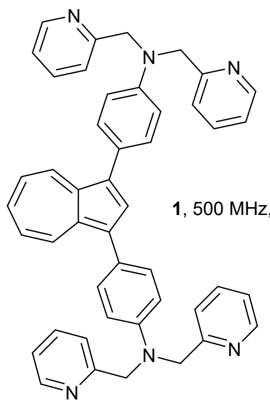




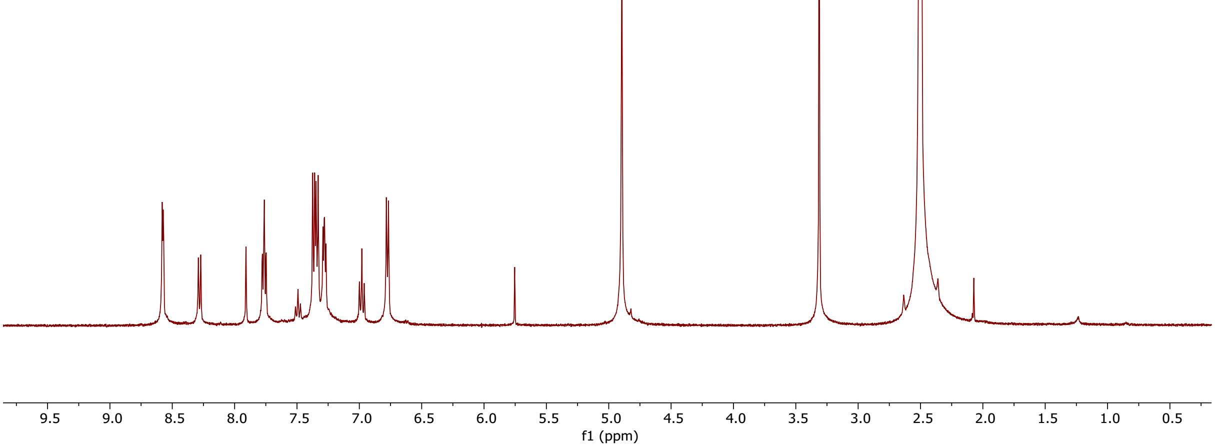
5, 300 MHz, $CDCl_3$

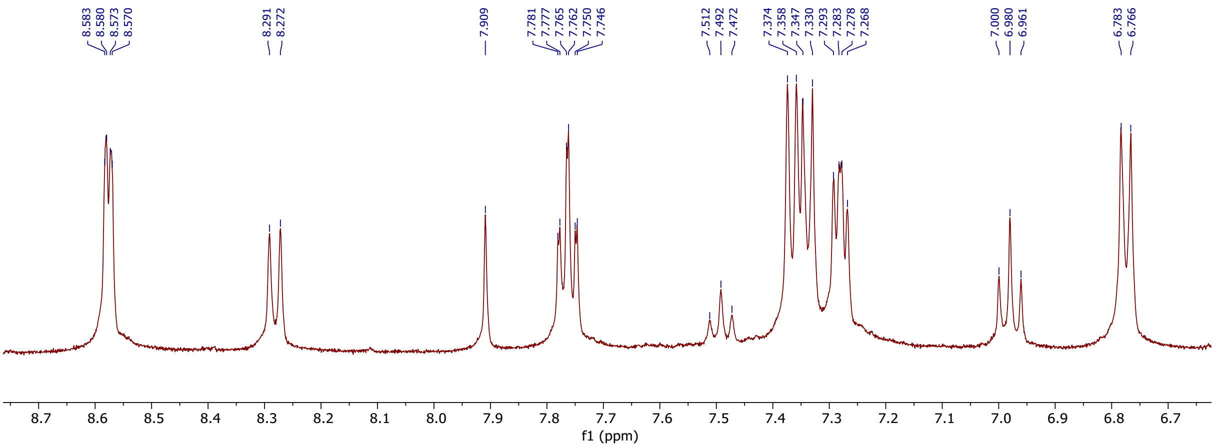


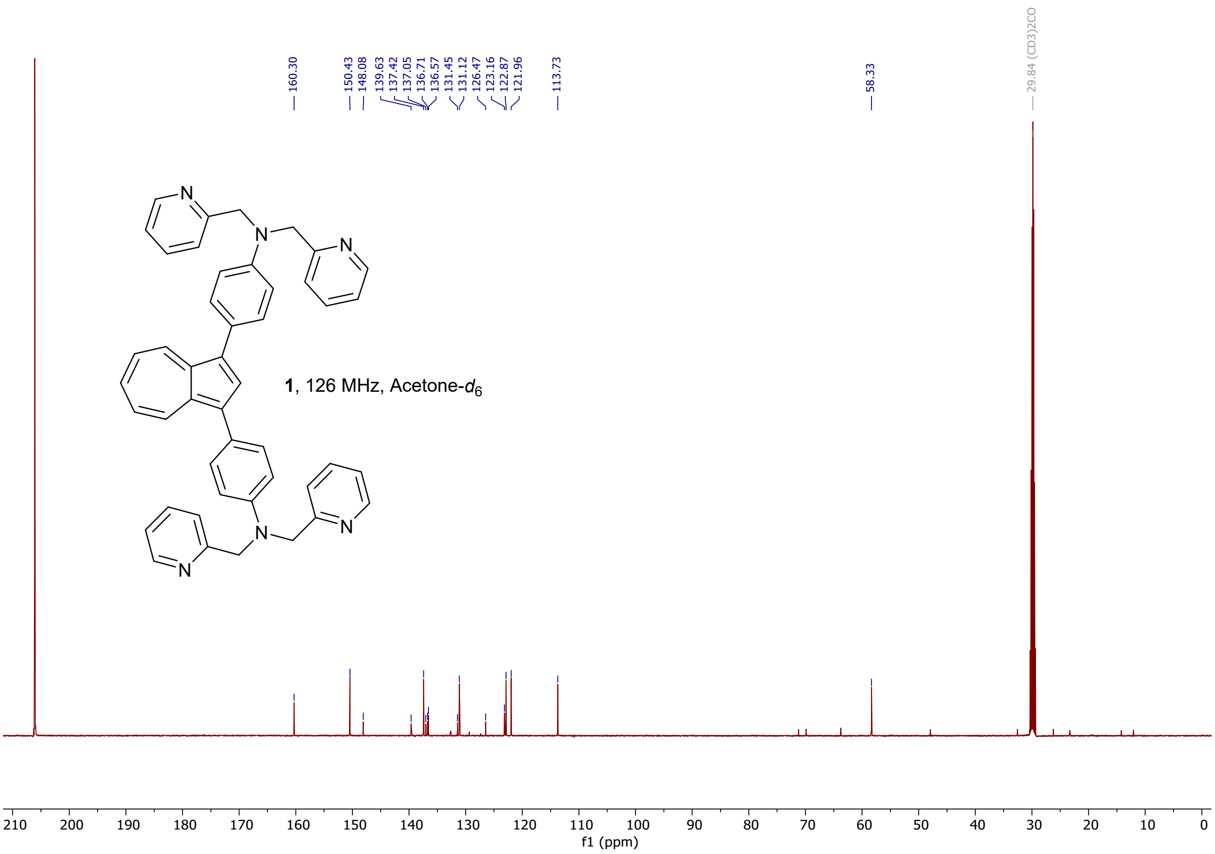


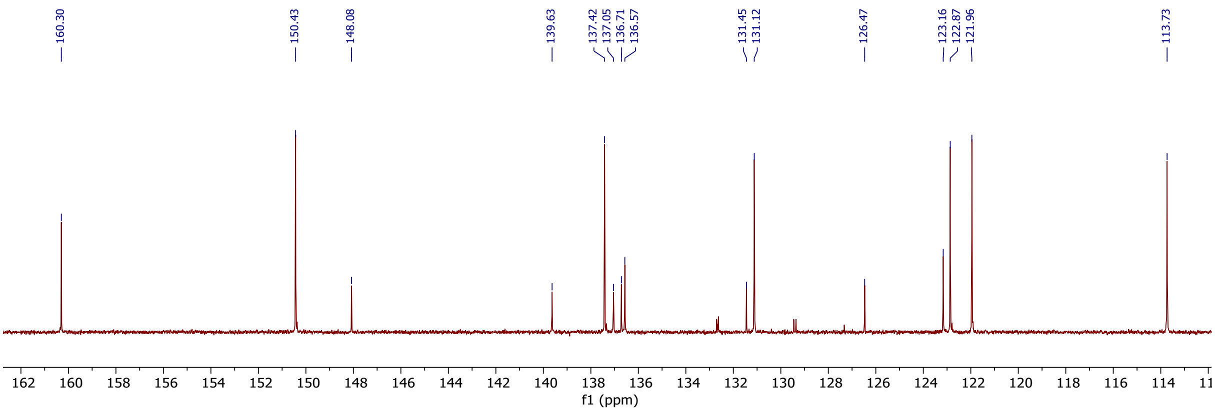


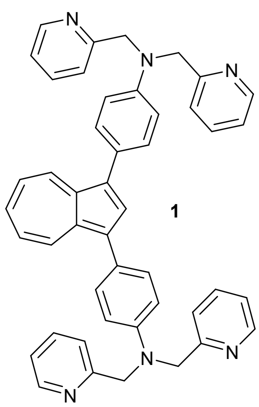
1, 500 MHz, DMSO-d_6



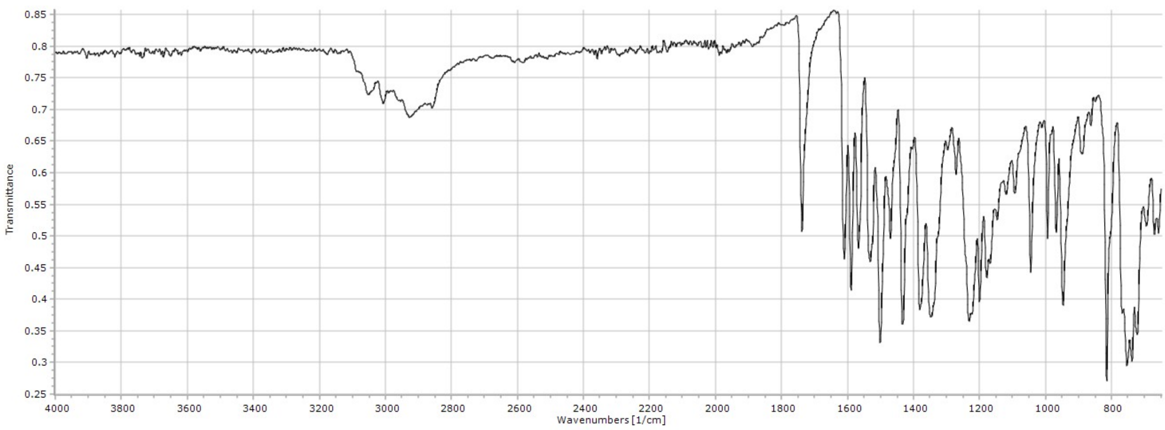



160.30
150.43
148.08
139.63
137.42
137.05
136.71
136.57
131.45
131.12
126.47
123.16
122.87
121.96
113.73
58.33
29.84 (CD3)2CO
1, 126 MHz, Acetone-d_6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

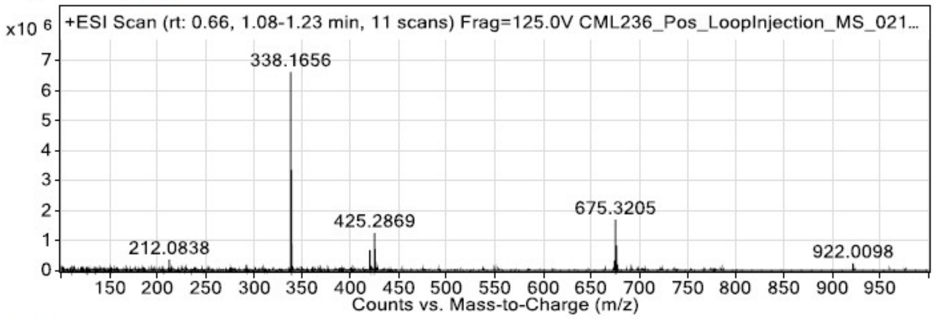

160.30
150.43
148.08
139.63
137.42
137.05
136.71
136.57
131.45
131.12
126.47
123.16
122.87
121.96
113.73
162 160 158 156 154 152 150 148 146 144 142 140 138 136 134 132 130 128 126 124 122 120 118 116 114 11
f1 (ppm)



1

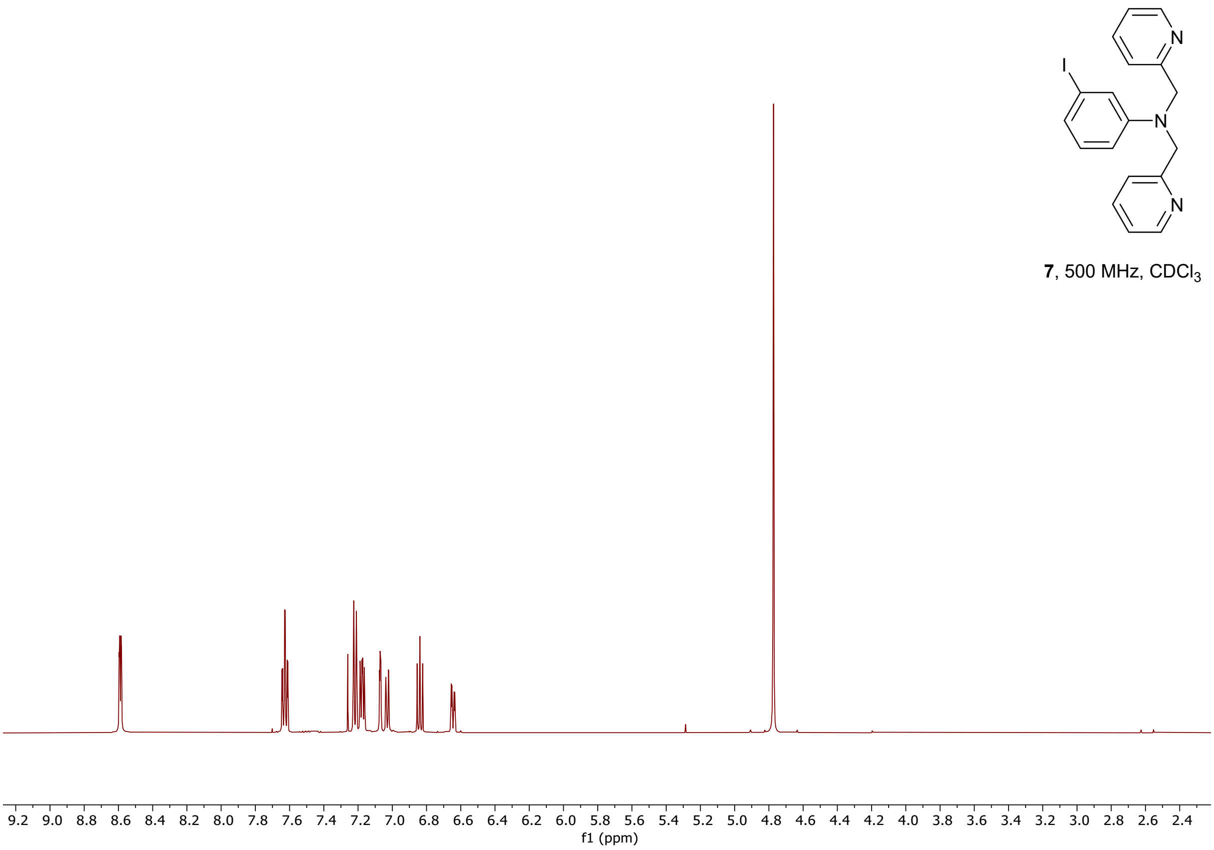


Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
Peak (1) in "+ BPC(all [-4]) Scan"	125	0	ESI

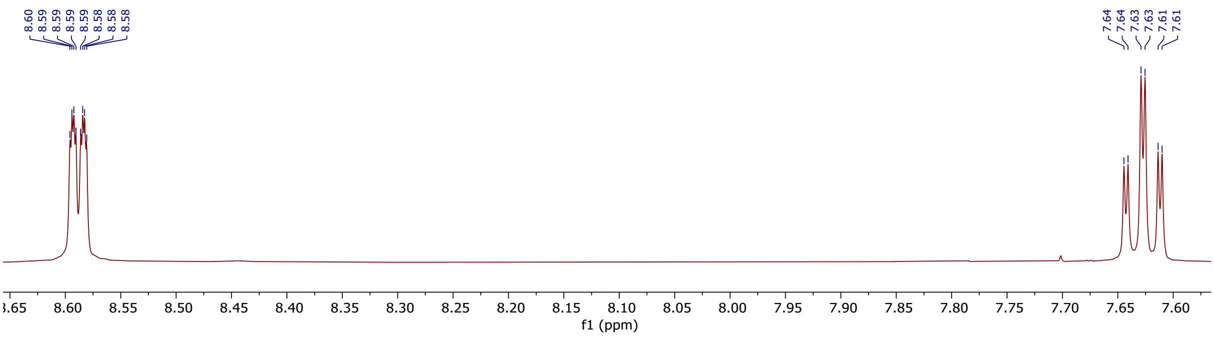


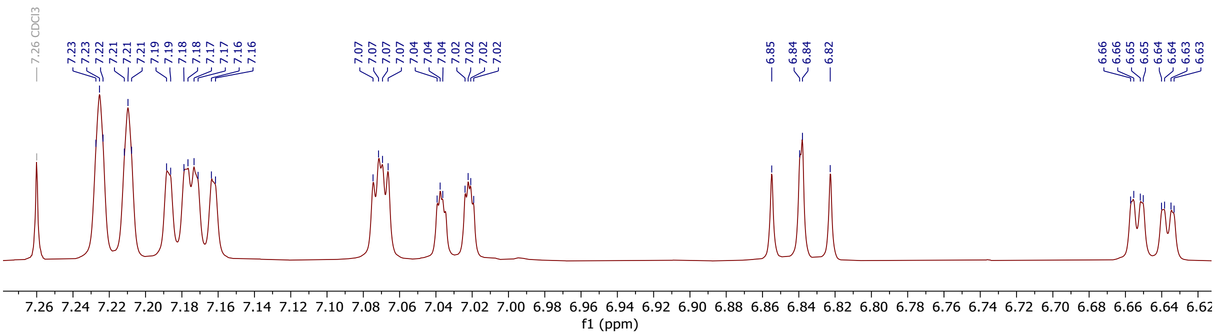
Peak List

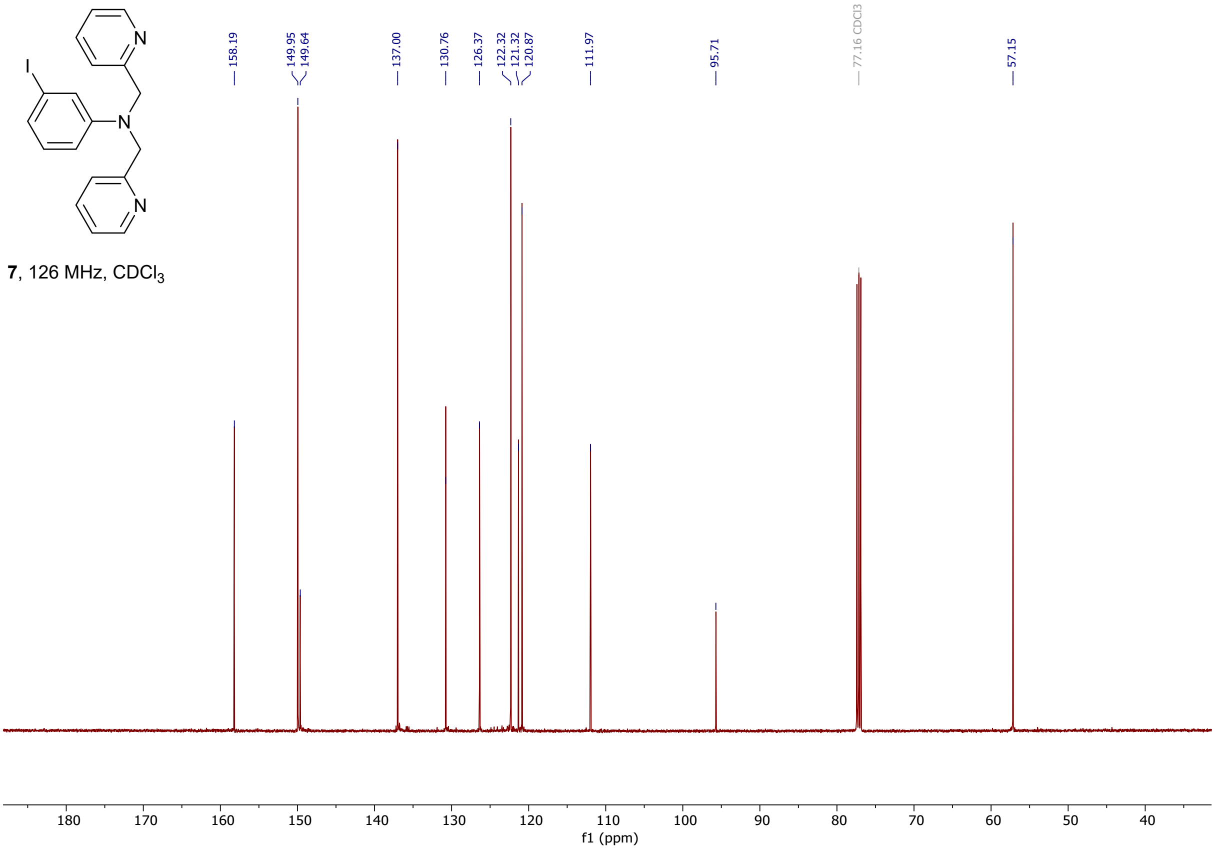
m/z	z	Abund
212.0838		370934.99
338.1656	2	6733966.59
338.667	2	3552150.66
339.1688	2	886451.62
420.3316	1	686079.36
425.2869	1	1258124.17
426.2903	1	296723.65
674.3131	1	340699.57
675.3205	1	1721116.73
676.3241	1	847936.95



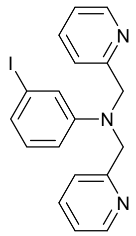
7, 500 MHz, $CDCl_3$



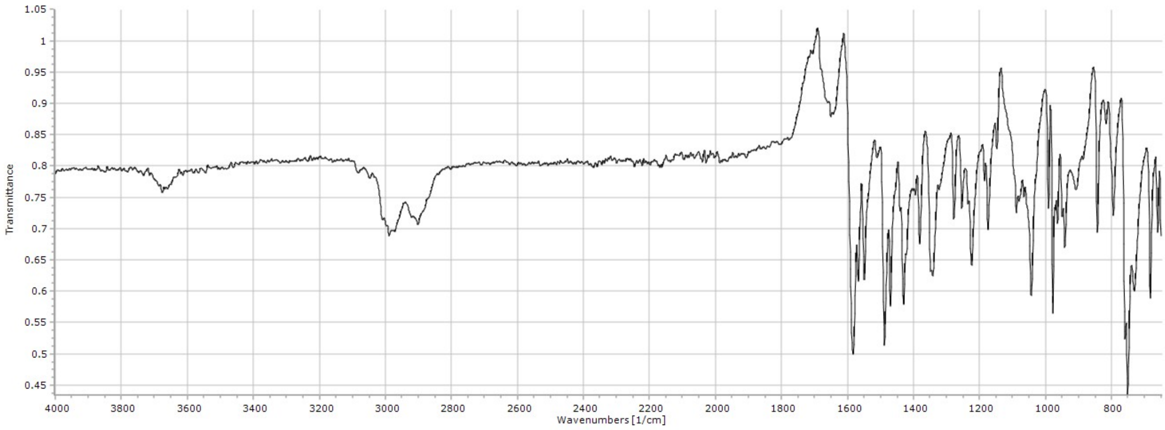




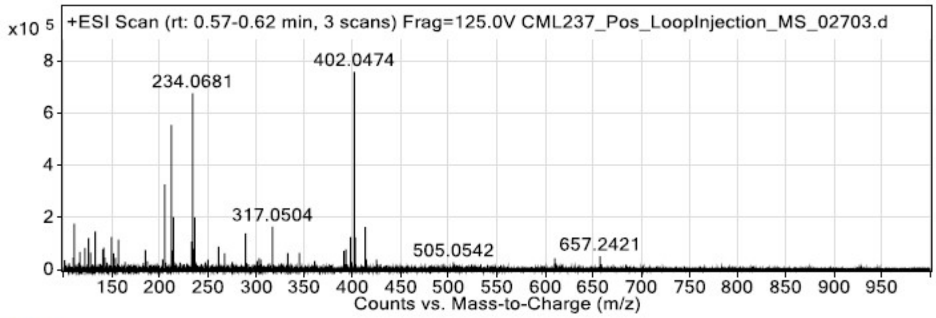
7, 126 MHz, $CDCl_3$



7

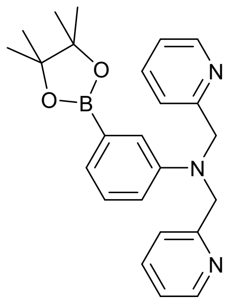


Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
Peak (1) in "+ BPC(all [-4]) Scan"	125	0	ESI

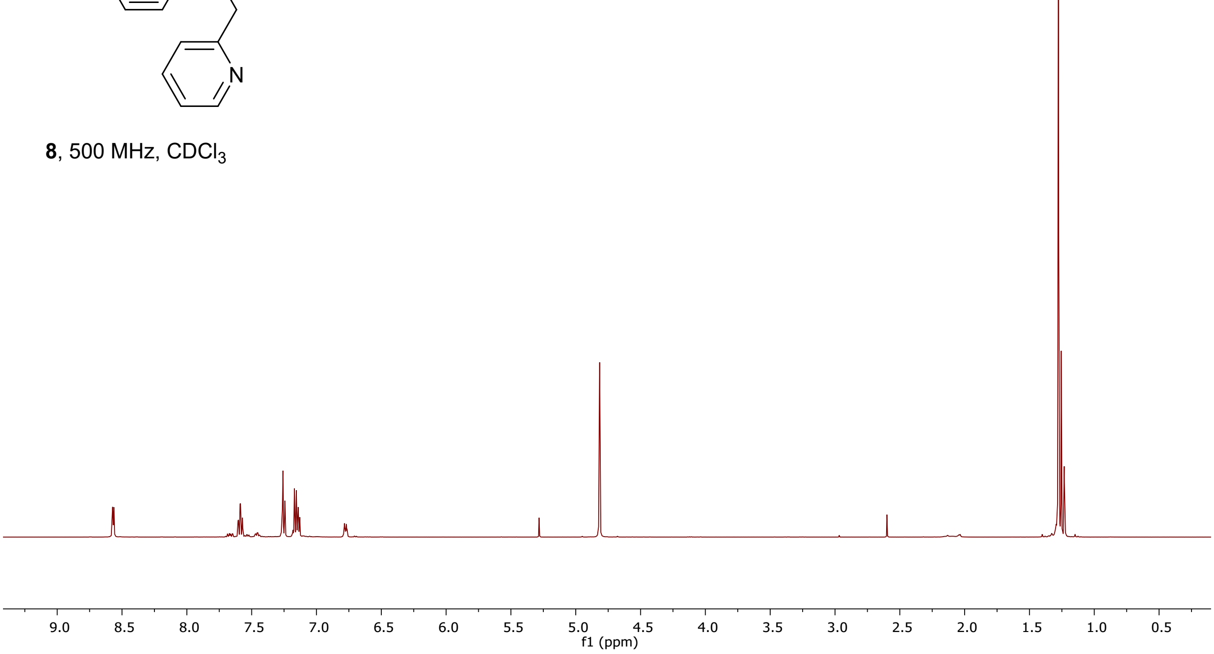


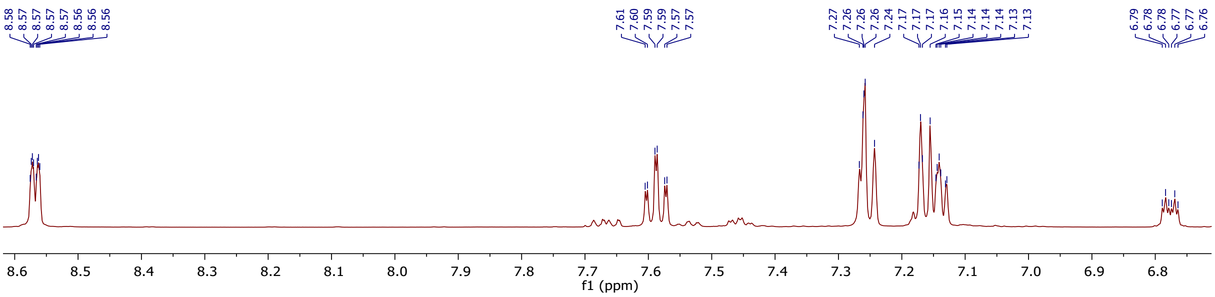
Peak List

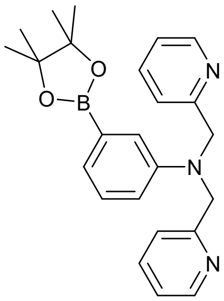
m/z	z	Abund
84.9615		340914.57
111.0224	1	180109.84
205.0705	1	348810.47
212.0861	1	571935.09
214.0832	1	202816.09
234.0681	1	680266.13
236.0652	1	208056.44
317.0504	1	164647.28
402.0474	1	795500.47
413.2681	1	163938.39



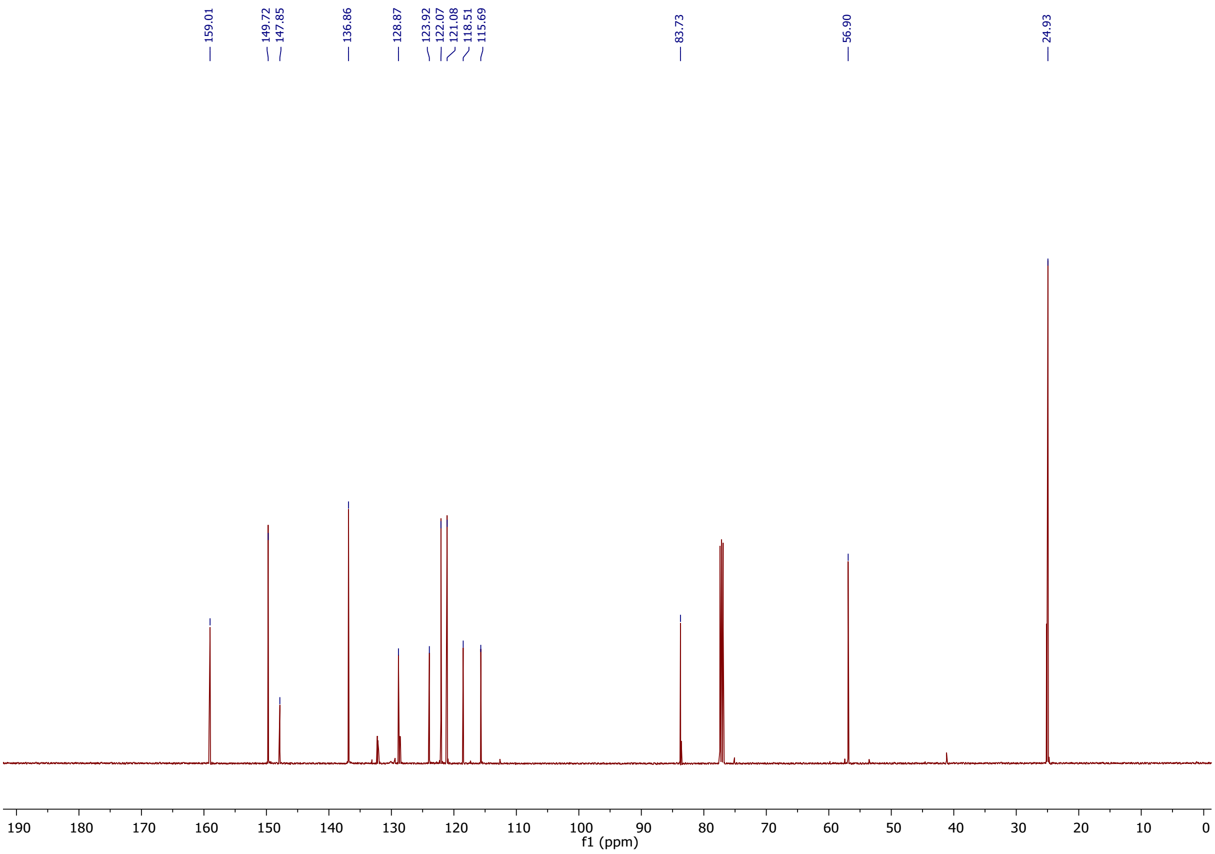
8, 500 MHz, $CDCl_3$

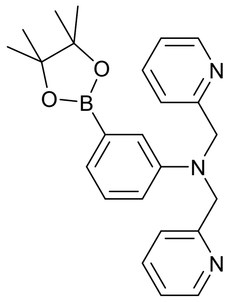




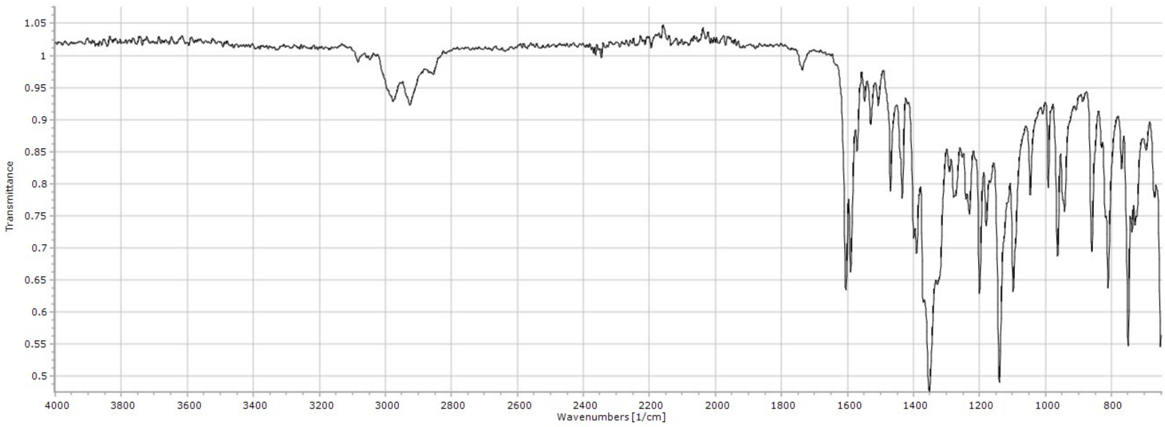


8, 126 MHz, $CDCl_3$

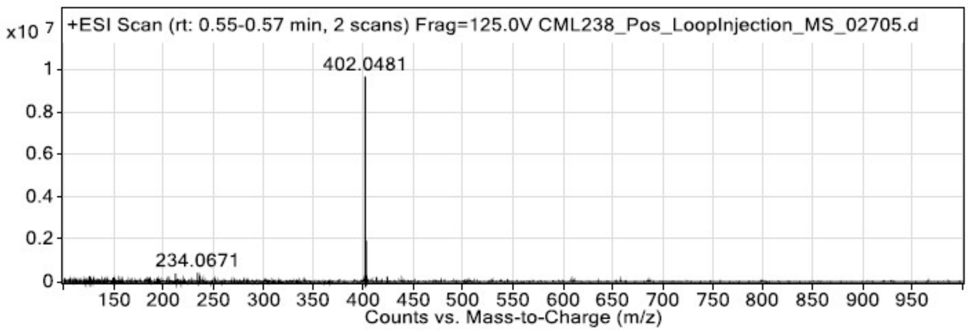




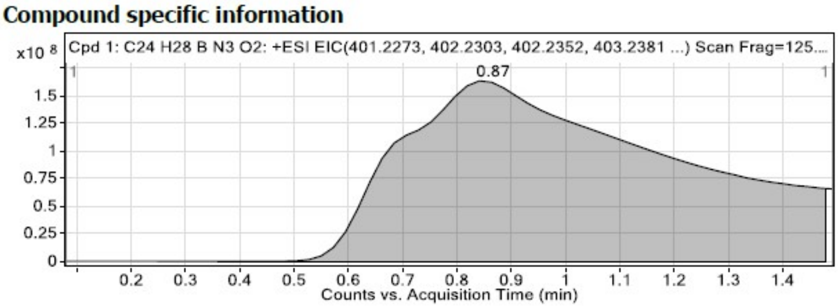
8



Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
Peak (1) in "+ BPC(all [-4]) Scan"	125	0	ESI

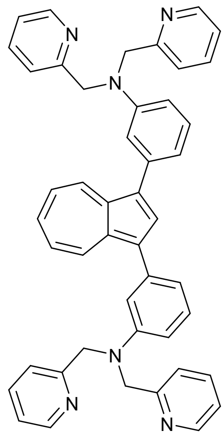


Compound specific information

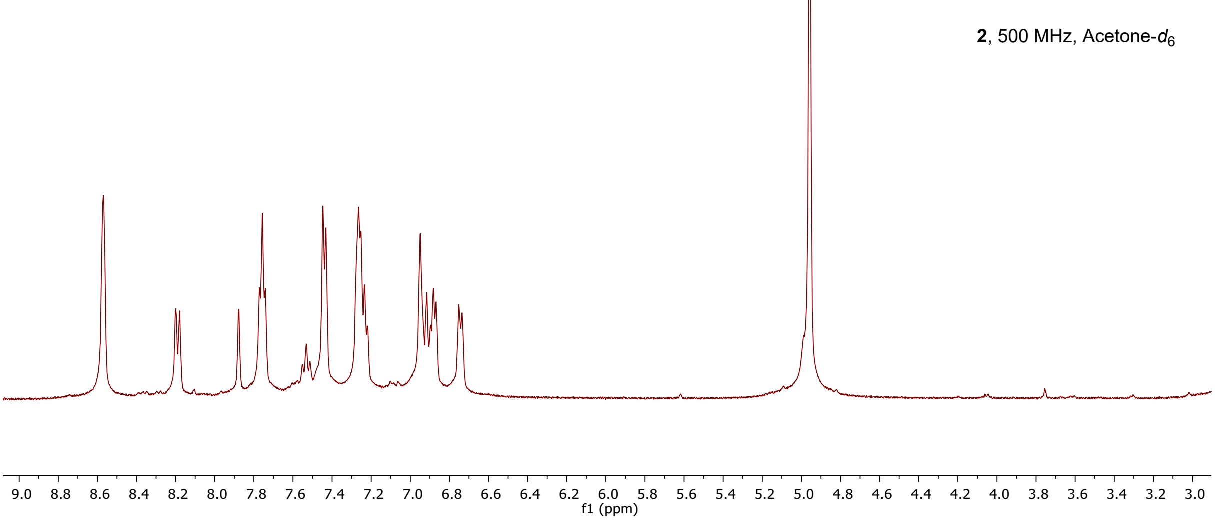


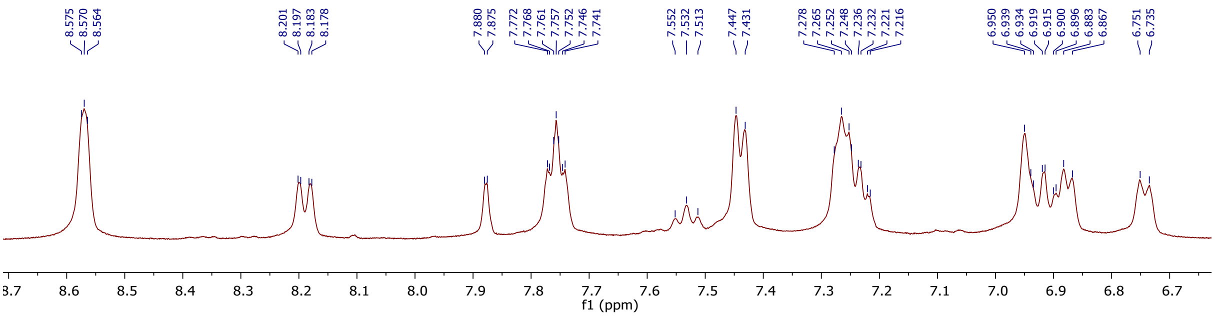
User Chromatogram Peak List

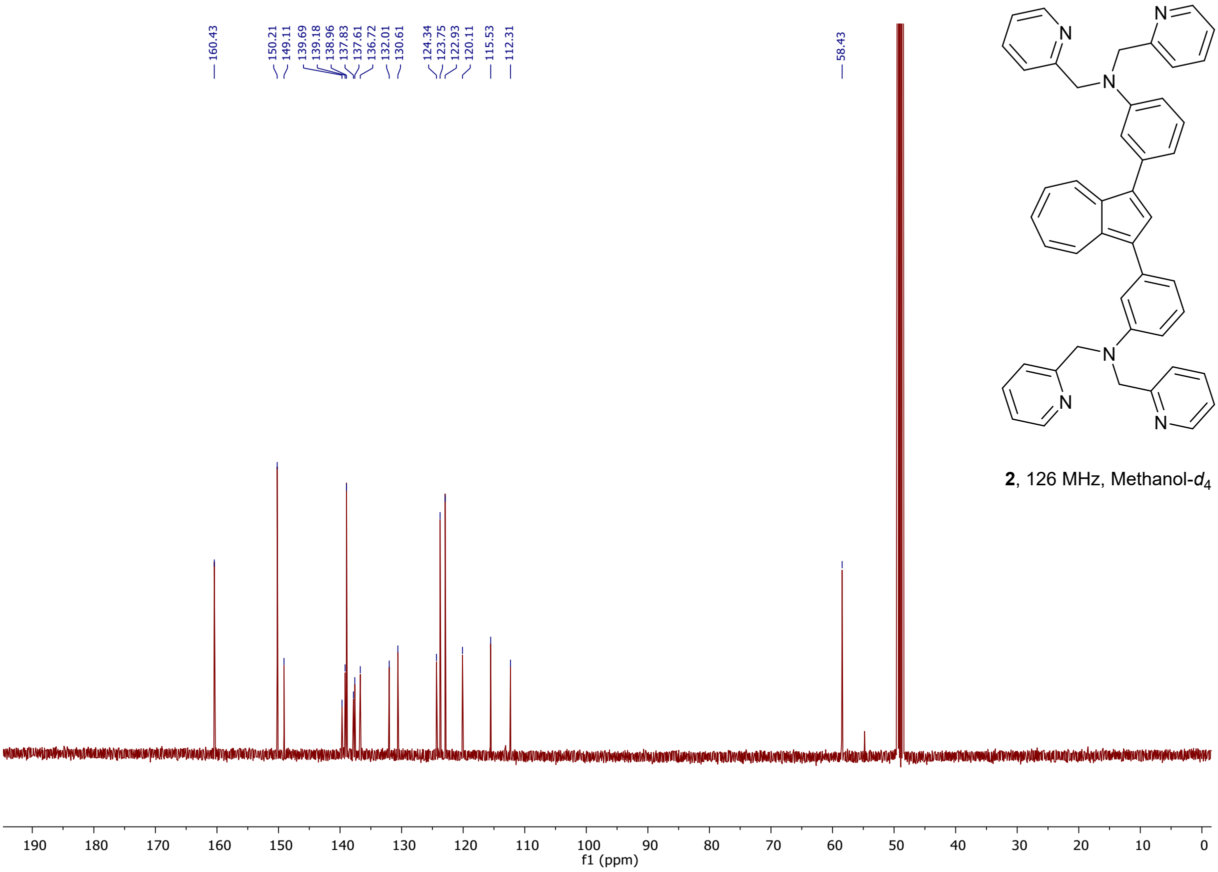
RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.88	453336124	100.00	100.00	402.2351	0.520



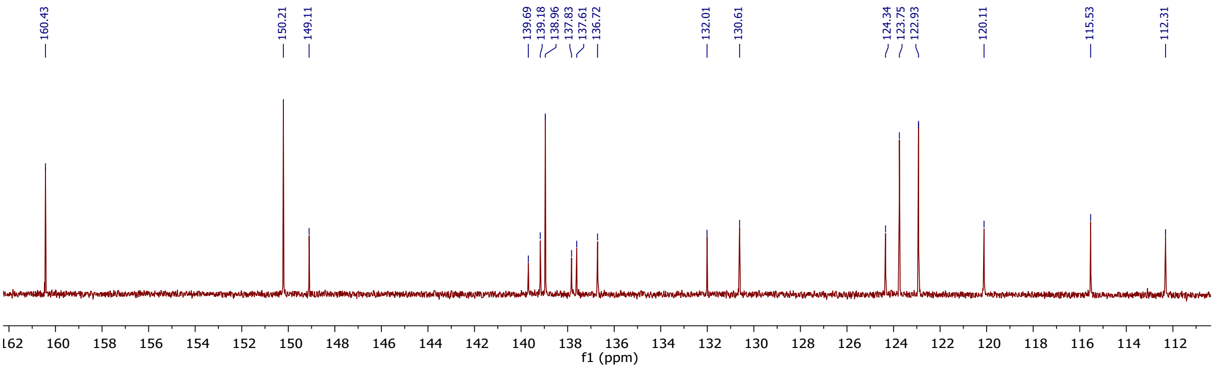
2, 500 MHz, Acetone-d_6

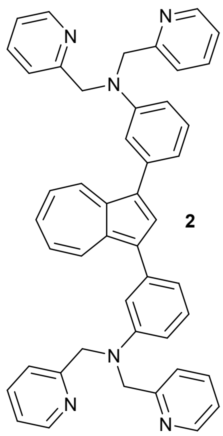




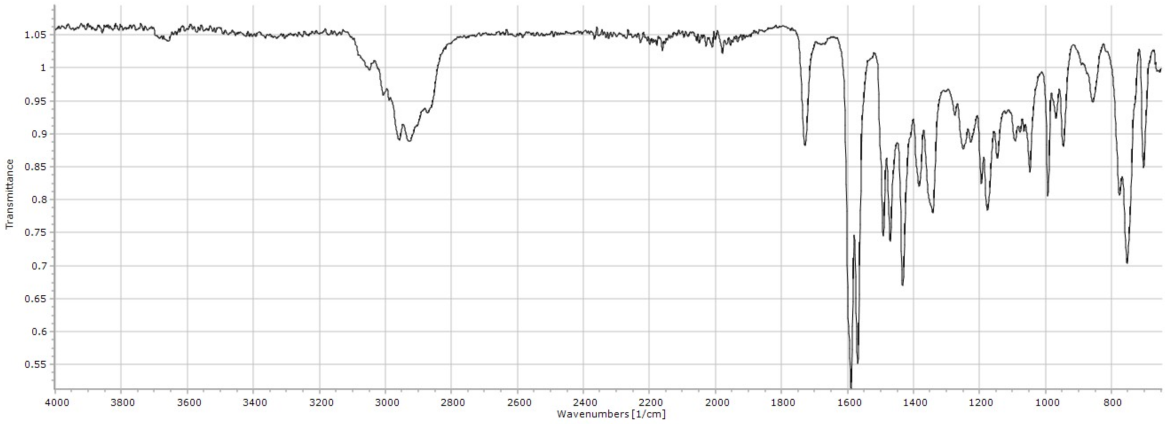


2, 126 MHz, Methanol-d_4

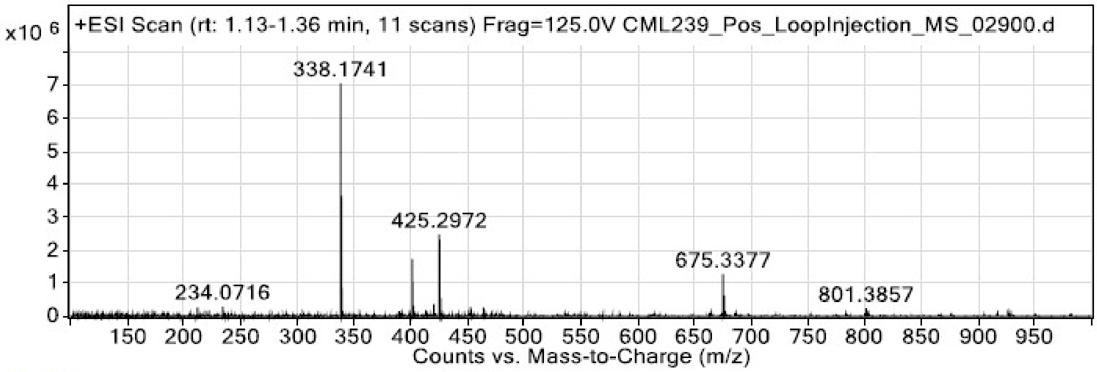




2



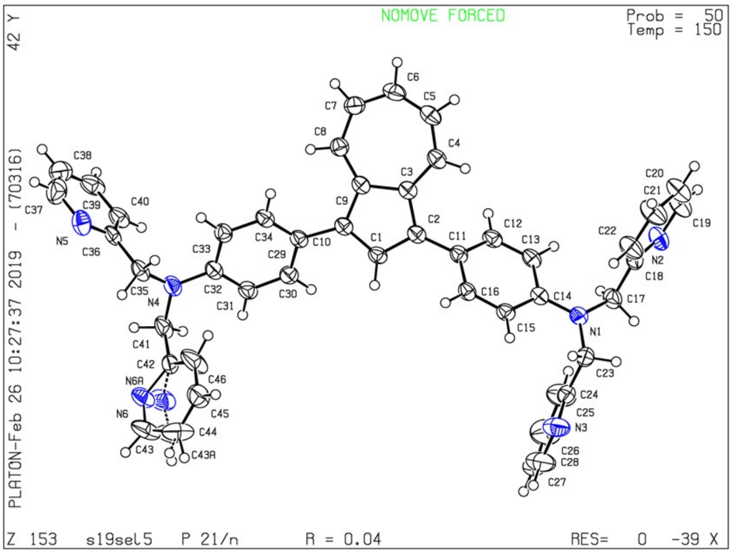
Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
Peak (1) in "+ BPC(all [-4]) Scan"	125	0	ESI

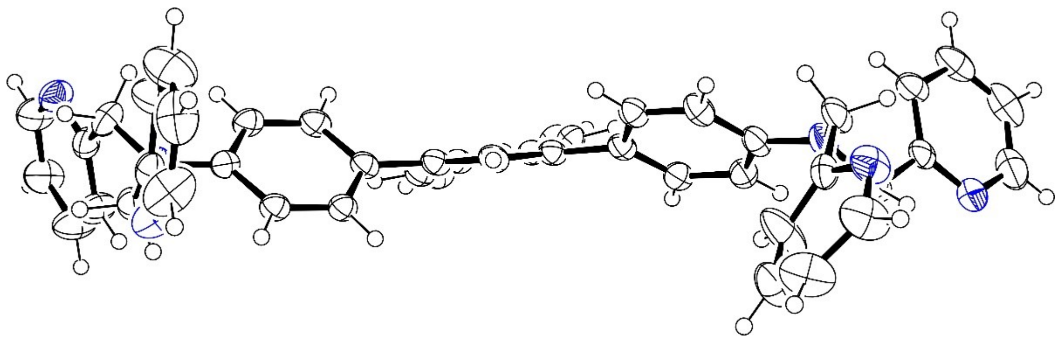


Peak List

m/z	z	Abund
338.1741	2	7075704.71
338.6755	2	3650049.72
339.1774	2	863190.13
401.1985	2	1772844
401.7003	2	1058551.49
420.3416	1	383217.18
425.2972	1	2501538.19
426.3009	1	553924.71
675.3377	1	1284119.39
676.3411	1	631124

X-Ray crystallographic data for **1**





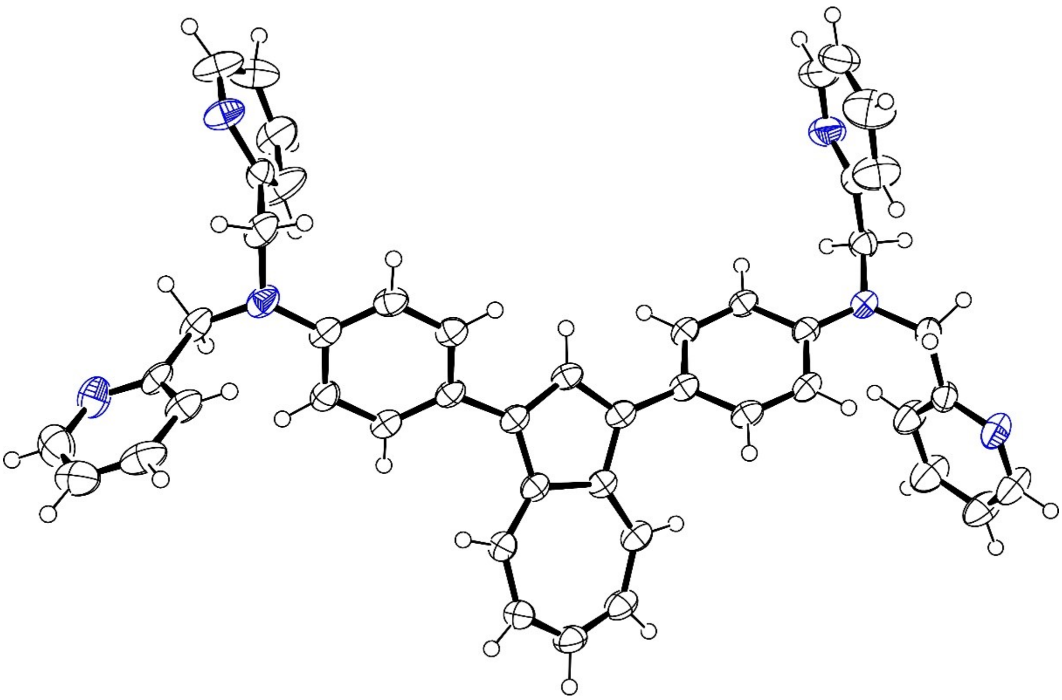


Table S1. Crystal data and structure refinement for **1**.

Identification code	s19sel5	
Empirical formula	$C_{46}H_{38}N_6$	
Formula weight	674.82	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 13.4530(2) Å	α= 90°.
	b = 8.67130(10) Å	β= 90.0660(9)°.
	c = 30.2422(3) Å	γ = 90°.
Volume	3527.90(8) $Å^3$	
Z	4	
Density (calculated)	1.271 Mg/m^3	
Absorption coefficient	0.589 mm^{-1}	
F(000)	1424	
Crystal size	0.385 x 0.139 x 0.032 mm^3	
Theta range for data collection	2.922 to 72.940°.	
Index ranges	-16<=h<=16, -10<=k<=6, -37<=l<=37	
Reflections collected	32405	
Independent reflections	7022 [R(int) = 0.0350]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.670	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7022 / 0 / 488	
Goodness-of-fit on F^2	1.061	
Final R indices [I>2sigma(I)]	R1 = 0.0444, wR2 = 0.1087	
R indices (all data)	R1 = 0.0551, wR2 = 0.1147	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.223 and -0.274 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	2165(1)	11510(2)	3740(1)	38(1)
N(2)	-251(1)	11594(2)	4307(1)	46(1)
N(3)	3715(1)	13302(2)	2901(1)	58(1)
N(4)	8034(1)	28(2)	3178(1)	40(1)
N(5)	9551(1)	-2847(2)	3771(1)	49(1)
C(1)	4828(1)	5128(2)	3888(1)	32(1)
C(2)	4123(1)	5850(2)	4158(1)	32(1)
C(3)	3963(1)	4872(2)	4527(1)	31(1)
C(4)	3424(1)	5252(2)	4901(1)	36(1)
C(5)	3251(1)	4377(2)	5280(1)	41(1)
C(6)	3508(1)	2864(2)	5362(1)	44(1)
C(7)	4031(1)	1832(2)	5099(1)	43(1)
C(8)	4520(1)	2105(2)	4700(1)	35(1)
C(9)	4568(1)	3452(2)	4454(1)	31(1)
C(10)	5108(1)	3687(2)	4059(1)	31(1)
C(11)	3627(1)	7327(2)	4067(1)	31(1)
C(12)	2596(1)	7500(2)	4109(1)	35(1)
C(13)	2114(1)	8862(2)	4005(1)	36(1)
C(14)	2641(1)	10140(2)	3844(1)	32(1)
C(15)	3676(1)	9973(2)	3797(1)	32(1)
C(16)	4146(1)	8613(2)	3913(1)	32(1)
C(17)	1094(1)	11631(2)	3785(1)	41(1)
C(18)	724(1)	11829(2)	4256(1)	37(1)
C(19)	-630(1)	11789(3)	4711(1)	55(1)
C(20)	-84(1)	12200(3)	5075(1)	56(1)
C(21)	921(1)	12432(3)	5019(1)	60(1)
C(22)	1336(1)	12243(2)	4604(1)	50(1)
C(23)	2698(1)	12767(2)	3531(1)	38(1)
C(24)	2923(1)	12541(2)	3043(1)	38(1)
C(25)	2333(2)	11677(3)	2766(1)	64(1)
C(26)	2577(2)	11610(3)	2317(1)	78(1)
C(27)	3409(2)	12380(3)	2172(1)	66(1)
C(28)	3944(2)	13197(3)	2474(1)	71(1)
C(29)	5828(1)	2648(2)	3845(1)	31(1)
C(30)	5894(1)	2627(2)	3382(1)	35(1)
C(31)	6606(1)	1769(2)	3164(1)	38(1)
C(32)	7296(1)	867(2)	3395(1)	35(1)
C(33)	7215(1)	840(2)	3860(1)	35(1)
C(34)	6504(1)	1728(2)	4074(1)	34(1)
C(35)	8870(1)	-591(2)	3424(1)	39(1)
C(36)	8759(1)	-2248(2)	3564(1)	35(1)
C(37)	9484(2)	-4308(2)	3906(1)	60(1)
C(38)	8665(2)	-5225(2)	3845(1)	59(1)
C(39)	7860(2)	-4604(2)	3628(1)	53(1)
C(40)	7900(1)	-3091(2)	3483(1)	41(1)
C(41)	8210(1)	225(2)	2708(1)	44(1)
C(42)	8873(1)	1582(2)	2595(1)	37(1)
C(43)	10088(6)	2477(9)	2126(2)	64(2)
N(6)	9446(5)	1352(7)	2226(2)	49(1)
C(43A)	9579(14)	3042(14)	2082(2)	74(3)
N(6A)	9062(11)	1786(14)	2198(2)	60(2)
C(44)	10104(2)	3919(3)	2363(1)	69(1)
C(45)	9657(2)	3986(2)	2757(1)	60(1)
C(46)	9039(2)	2788(2)	2878(1)	75(1)

Table S3. Bond lengths [Å] for **1**.

N(1)-C(14)	1.385(2)	C(22)-H(22)	0.9500
N(1)-C(23)	1.450(2)	C(23)-C(24)	1.518(2)
N(1)-C(17)	1.4503(19)	C(23)-H(23A)	0.9900
N(2)-C(19)	1.336(2)	C(23)-H(23B)	0.9900
N(2)-C(18)	1.336(2)	C(24)-C(25)	1.375(3)
N(3)-C(24)	1.326(2)	C(25)-C(26)	1.397(3)
N(3)-C(28)	1.331(3)	C(25)-H(25)	0.9500
N(4)-C(32)	1.3957(19)	C(26)-C(27)	1.376(4)
N(4)-C(41)	1.451(2)	C(26)-H(26)	0.9500
N(4)-C(35)	1.451(2)	C(27)-C(28)	1.360(3)
N(5)-C(37)	1.334(3)	C(27)-H(27)	0.9500
N(5)-C(36)	1.341(2)	C(28)-H(28)	0.9500
C(1)-C(2)	1.400(2)	C(29)-C(34)	1.394(2)
C(1)-C(10)	1.403(2)	C(29)-C(30)	1.401(2)
C(1)-H(1)	0.9500	C(30)-C(31)	1.381(2)
C(2)-C(3)	1.419(2)	C(30)-H(30)	0.9500
C(2)-C(11)	1.470(2)	C(31)-C(32)	1.400(2)
C(3)-C(4)	1.384(2)	C(31)-H(31)	0.9500
C(3)-C(9)	1.492(2)	C(32)-C(33)	1.409(2)
C(4)-C(5)	1.395(2)	C(33)-C(34)	1.390(2)
C(4)-H(4)	0.9500	C(33)-H(33)	0.9500
C(5)-C(6)	1.379(3)	C(34)-H(34)	0.9500
C(5)-H(5)	0.9500	C(35)-C(36)	1.505(2)
C(6)-C(7)	1.389(2)	C(35)-H(35A)	0.9900
C(6)-H(6)	0.9500	C(35)-H(35B)	0.9900
C(7)-C(8)	1.396(2)	C(36)-C(40)	1.388(2)
C(7)-H(7)	0.9500	C(37)-C(38)	1.372(3)
C(8)-C(9)	1.386(2)	C(37)-H(37)	0.9500
C(8)-H(8)	0.9500	C(38)-C(39)	1.375(3)
C(9)-C(10)	1.4123(19)	C(38)-H(38)	0.9500
C(10)-C(29)	1.4747(19)	C(39)-C(40)	1.384(3)
C(11)-C(16)	1.397(2)	C(39)-H(39)	0.9500
C(11)-C(12)	1.401(2)	C(40)-H(40)	0.9500
C(12)-C(13)	1.384(2)	C(41)-C(42)	1.516(2)
C(12)-H(12)	0.9500	C(41)-H(41A)	0.9900
C(13)-C(14)	1.404(2)	C(41)-H(41B)	0.9900
C(13)-H(13)	0.9500	C(42)-N(6A)	1.243(7)
C(14)-C(15)	1.4073(19)	C(42)-C(46)	1.368(3)
C(15)-C(16)	1.383(2)	C(42)-N(6)	1.373(5)
C(15)-H(15)	0.9500	C(43)-N(6)	1.338(6)
C(16)-H(16)	0.9500	C(43)-C(44)	1.441(7)
C(17)-C(18)	1.518(2)	C(43)-H(43)	0.9500
C(17)-H(17A)	0.9900	C(43A)-N(6A)	1.339(12)
C(17)-H(17B)	0.9900	C(43A)-C(44)	1.341(10)
C(18)-C(22)	1.384(2)	C(43A)-H(43A)	0.9500
C(19)-C(20)	1.370(3)	C(44)-C(45)	1.337(3)
C(19)-H(19)	0.9500	C(44)-H(44)	0.9500
C(20)-C(21)	1.377(3)	C(44)-H(44A)	0.9500
C(20)-H(20)	0.9500	C(45)-C(46)	1.380(3)
C(21)-C(22)	1.384(3)	C(45)-H(45)	0.9500
C(21)-H(21)	0.9500	C(46)-H(46)	0.9500

Table S4. Bond angles [°] for **1**.

C(14)-N(1)-C(23)	120.94(12)	N(1)-C(17)-H(17A)	108.5
C(14)-N(1)-C(17)	119.96(13)	C(18)-C(17)-H(17A)	108.5
C(23)-N(1)-C(17)	118.61(13)	N(1)-C(17)-H(17B)	108.5
C(19)-N(2)-C(18)	117.57(15)	C(18)-C(17)-H(17B)	108.5
C(24)-N(3)-C(28)	117.98(19)	H(17A)-C(17)-H(17B)	107.5
C(32)-N(4)-C(41)	121.06(14)	N(2)-C(18)-C(22)	122.31(15)
C(32)-N(4)-C(35)	120.19(13)	N(2)-C(18)-C(17)	114.53(14)
C(41)-N(4)-C(35)	114.81(13)	C(22)-C(18)-C(17)	123.14(14)
C(37)-N(5)-C(36)	117.27(17)	N(2)-C(19)-C(20)	124.23(16)
C(2)-C(1)-C(10)	111.38(13)	N(2)-C(19)-H(19)	117.9
C(2)-C(1)-H(1)	124.3	C(20)-C(19)-H(19)	117.9
C(10)-C(1)-H(1)	124.3	C(19)-C(20)-C(21)	117.74(17)
C(1)-C(2)-C(3)	107.14(13)	C(19)-C(20)-H(20)	121.1
C(1)-C(2)-C(11)	126.12(13)	C(21)-C(20)-H(20)	121.1
C(3)-C(2)-C(11)	126.73(13)	C(20)-C(21)-C(22)	119.42(17)
C(4)-C(3)-C(2)	125.51(14)	C(20)-C(21)-H(21)	120.3
C(4)-C(3)-C(9)	127.16(14)	C(22)-C(21)-H(21)	120.3
C(2)-C(3)-C(9)	107.05(12)	C(18)-C(22)-C(21)	118.73(16)
C(3)-C(4)-C(5)	129.07(15)	C(18)-C(22)-H(22)	120.6
C(3)-C(4)-H(4)	115.5	C(21)-C(22)-H(22)	120.6
C(5)-C(4)-H(4)	115.5	N(1)-C(23)-C(24)	115.15(13)
C(6)-C(5)-C(4)	128.54(15)	N(1)-C(23)-H(23A)	108.5
C(6)-C(5)-H(5)	115.7	C(24)-C(23)-H(23A)	108.5
C(4)-C(5)-H(5)	115.7	N(1)-C(23)-H(23B)	108.5
C(5)-C(6)-C(7)	129.59(15)	C(24)-C(23)-H(23B)	108.5
C(5)-C(6)-H(6)	115.2	H(23A)-C(23)-H(23B)	107.5
C(7)-C(6)-H(6)	115.2	N(3)-C(24)-C(25)	122.34(17)
C(6)-C(7)-C(8)	128.71(16)	N(3)-C(24)-C(23)	114.39(15)
C(6)-C(7)-H(7)	115.6	C(25)-C(24)-C(23)	123.22(15)
C(8)-C(7)-H(7)	115.6	C(24)-C(25)-C(26)	118.7(2)
C(9)-C(8)-C(7)	128.99(15)	C(24)-C(25)-H(25)	120.7
C(9)-C(8)-H(8)	115.5	C(26)-C(25)-H(25)	120.7
C(7)-C(8)-H(8)	115.5	C(27)-C(26)-C(25)	118.8(2)
C(8)-C(9)-C(10)	126.80(14)	C(27)-C(26)-H(26)	120.6
C(8)-C(9)-C(3)	126.15(13)	C(25)-C(26)-H(26)	120.6
C(10)-C(9)-C(3)	106.70(13)	C(28)-C(27)-C(26)	118.0(2)
C(1)-C(10)-C(9)	107.61(13)	C(28)-C(27)-H(27)	121.0
C(1)-C(10)-C(29)	123.88(13)	C(26)-C(27)-H(27)	121.0
C(9)-C(10)-C(29)	128.50(14)	N(3)-C(28)-C(27)	124.2(2)
C(16)-C(11)-C(12)	116.14(14)	N(3)-C(28)-H(28)	117.9
C(16)-C(11)-C(2)	122.07(13)	C(27)-C(28)-H(28)	117.9
C(12)-C(11)-C(2)	121.71(13)	C(34)-C(29)-C(30)	116.56(13)
C(13)-C(12)-C(11)	122.31(13)	C(34)-C(29)-C(10)	124.02(13)
C(13)-C(12)-H(12)	118.8	C(30)-C(29)-C(10)	119.31(13)
C(11)-C(12)-H(12)	118.8	C(31)-C(30)-C(29)	121.93(15)
C(12)-C(13)-C(14)	121.10(13)	C(31)-C(30)-H(30)	119.0
C(12)-C(13)-H(13)	119.4	C(29)-C(30)-H(30)	119.0
C(14)-C(13)-H(13)	119.4	C(30)-C(31)-C(32)	121.45(14)
N(1)-C(14)-C(13)	121.48(13)	C(30)-C(31)-H(31)	119.3
N(1)-C(14)-C(15)	121.54(13)	C(32)-C(31)-H(31)	119.3
C(13)-C(14)-C(15)	116.98(14)	N(4)-C(32)-C(31)	121.88(14)
C(16)-C(15)-C(14)	121.01(13)	N(4)-C(32)-C(33)	121.03(15)
C(16)-C(15)-H(15)	119.5	C(31)-C(32)-C(33)	117.08(13)
C(14)-C(15)-H(15)	119.5	C(34)-C(33)-C(32)	120.66(14)
C(15)-C(16)-C(11)	122.44(13)	C(34)-C(33)-H(33)	119.7
C(15)-C(16)-H(16)	118.8	C(32)-C(33)-H(33)	119.7
C(11)-C(16)-H(16)	118.8	C(33)-C(34)-C(29)	122.26(14)
N(1)-C(17)-C(18)	115.13(13)	C(33)-C(34)-H(34)	118.9

C(29)-C(34)-H(34)	118.9	H(41A)-C(41)-H(41B)	107.6
N(4)-C(35)-C(36)	114.80(13)	N(6A)-C(42)-C(46)	117.5(5)
N(4)-C(35)-H(35A)	108.6	C(46)-C(42)-N(6)	121.8(2)
C(36)-C(35)-H(35A)	108.6	N(6A)-C(42)-C(41)	116.7(4)
N(4)-C(35)-H(35B)	108.6	C(46)-C(42)-C(41)	123.32(15)
C(36)-C(35)-H(35B)	108.6	N(6)-C(42)-C(41)	113.7(2)
H(35A)-C(35)-H(35B)	107.5	N(6)-C(43)-C(44)	122.0(4)
N(5)-C(36)-C(40)	122.55(16)	N(6)-C(43)-H(43)	119.0
N(5)-C(36)-C(35)	114.95(14)	C(44)-C(43)-H(43)	119.0
C(40)-C(36)-C(35)	122.50(15)	C(43)-N(6)-C(42)	116.2(4)
N(5)-C(37)-C(38)	124.2(2)	N(6A)-C(43A)-C(44)	124.6(6)
N(5)-C(37)-H(37)	117.9	N(6A)-C(43A)-H(43A)	117.7
C(38)-C(37)-H(37)	117.9	C(44)-C(43A)-H(43A)	117.7
C(37)-C(38)-C(39)	118.07(18)	C(42)-N(6A)-C(43A)	118.5(7)
C(37)-C(38)-H(38)	121.0	C(45)-C(44)-C(43A)	110.7(5)
C(39)-C(38)-H(38)	121.0	C(45)-C(44)-C(43)	118.3(2)
C(38)-C(39)-C(40)	119.35(18)	C(45)-C(44)-H(44)	120.8
C(38)-C(39)-H(39)	120.3	C(43)-C(44)-H(44)	120.8
C(40)-C(39)-H(39)	120.3	C(45)-C(44)-H(44A)	124.6
C(39)-C(40)-C(36)	118.52(18)	C(43A)-C(44)-H(44A)	124.6
C(39)-C(40)-H(40)	120.7	C(44)-C(45)-C(46)	118.3(2)
C(36)-C(40)-H(40)	120.7	C(44)-C(45)-H(45)	120.9
N(4)-C(41)-C(42)	114.04(13)	C(46)-C(45)-H(45)	120.9
N(4)-C(41)-H(41A)	108.7	C(42)-C(46)-C(45)	120.63(18)
C(42)-C(41)-H(41A)	108.7	C(42)-C(46)-H(46)	119.7
N(4)-C(41)-H(41B)	108.7	C(45)-C(46)-H(46)	119.7
C(42)-C(41)-H(41B)	108.7		

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters ($Å^2$x 10^3) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	31(1)	44(1)	40(1)	6(1)	6(1)	3(1)
N(2)	30(1)	60(1)	48(1)	-10(1)	4(1)	2(1)
N(3)	45(1)	78(1)	50(1)	20(1)	2(1)	-10(1)
N(4)	42(1)	34(1)	46(1)	-8(1)	14(1)	0(1)
N(5)	45(1)	46(1)	57(1)	-16(1)	2(1)	4(1)
C(1)	33(1)	32(1)	33(1)	-3(1)	7(1)	-7(1)
C(2)	31(1)	31(1)	34(1)	-5(1)	4(1)	-6(1)
C(3)	29(1)	32(1)	32(1)	-5(1)	1(1)	-6(1)
C(4)	35(1)	39(1)	34(1)	-9(1)	4(1)	-4(1)
C(5)	38(1)	56(1)	30(1)	-7(1)	5(1)	-2(1)
C(6)	38(1)	65(1)	29(1)	7(1)	4(1)	-2(1)
C(7)	37(1)	50(1)	41(1)	12(1)	2(1)	1(1)
C(8)	30(1)	38(1)	37(1)	1(1)	1(1)	0(1)
C(9)	27(1)	35(1)	31(1)	-5(1)	1(1)	-4(1)
C(10)	28(1)	31(1)	34(1)	-4(1)	2(1)	-6(1)
C(11)	33(1)	30(1)	31(1)	-6(1)	4(1)	-3(1)
C(12)	32(1)	35(1)	38(1)	-3(1)	7(1)	-9(1)
C(13)	25(1)	43(1)	38(1)	-4(1)	6(1)	-4(1)
C(14)	29(1)	36(1)	29(1)	-3(1)	2(1)	-1(1)
C(15)	28(1)	33(1)	35(1)	-1(1)	4(1)	-6(1)
C(16)	26(1)	34(1)	36(1)	-4(1)	4(1)	-4(1)
C(17)	30(1)	55(1)	39(1)	3(1)	1(1)	8(1)
C(18)	31(1)	37(1)	42(1)	0(1)	3(1)	5(1)
C(19)	33(1)	74(1)	56(1)	-16(1)	12(1)	-4(1)
C(20)	47(1)	73(1)	48(1)	-16(1)	14(1)	-6(1)
C(21)	45(1)	89(2)	45(1)	-18(1)	3(1)	-10(1)
C(22)	33(1)	71(1)	47(1)	-9(1)	4(1)	-6(1)
C(23)	38(1)	34(1)	42(1)	1(1)	0(1)	3(1)
C(24)	37(1)	36(1)	42(1)	9(1)	1(1)	6(1)
C(25)	76(1)	68(1)	50(1)	-6(1)	6(1)	-23(1)
C(26)	111(2)	76(2)	49(1)	-11(1)	-1(1)	-14(1)
C(27)	88(2)	67(1)	43(1)	17(1)	15(1)	16(1)
C(28)	58(1)	102(2)	52(1)	25(1)	9(1)	-7(1)
C(29)	29(1)	29(1)	36(1)	-4(1)	7(1)	-7(1)
C(30)	36(1)	30(1)	37(1)	-2(1)	5(1)	-4(1)
C(31)	46(1)	32(1)	35(1)	-5(1)	10(1)	-3(1)
C(32)	36(1)	27(1)	43(1)	-7(1)	12(1)	-6(1)
C(33)	31(1)	33(1)	42(1)	-2(1)	6(1)	-2(1)
C(34)	31(1)	36(1)	34(1)	-3(1)	6(1)	-5(1)
C(35)	31(1)	35(1)	51(1)	-14(1)	13(1)	-7(1)
C(36)	33(1)	35(1)	38(1)	-14(1)	12(1)	-2(1)
C(37)	77(1)	47(1)	55(1)	-9(1)	0(1)	17(1)
C(38)	95(2)	37(1)	46(1)	-6(1)	20(1)	1(1)
C(39)	67(1)	44(1)	48(1)	-15(1)	24(1)	-20(1)
C(40)	40(1)	40(1)	44(1)	-13(1)	12(1)	-10(1)
C(41)	48(1)	39(1)	45(1)	-17(1)	13(1)	1(1)
C(42)	38(1)	38(1)	35(1)	-2(1)	4(1)	9(1)
C(43)	76(4)	79(4)	38(2)	-10(2)	26(2)	-19(3)
N(6)	56(2)	57(2)	32(1)	-10(1)	13(2)	-4(2)
C(43A)	106(9)	82(6)	33(3)	6(3)	27(4)	-5(6)
N(6A)	79(6)	69(5)	31(2)	-7(3)	9(3)	-4(4)
C(44)	89(2)	70(1)	47(1)	13(1)	8(1)	-28(1)
C(45)	67(1)	39(1)	74(1)	-9(1)	25(1)	-6(1)
C(46)	94(2)	50(1)	82(2)	-31(1)	56(1)	-25(1)

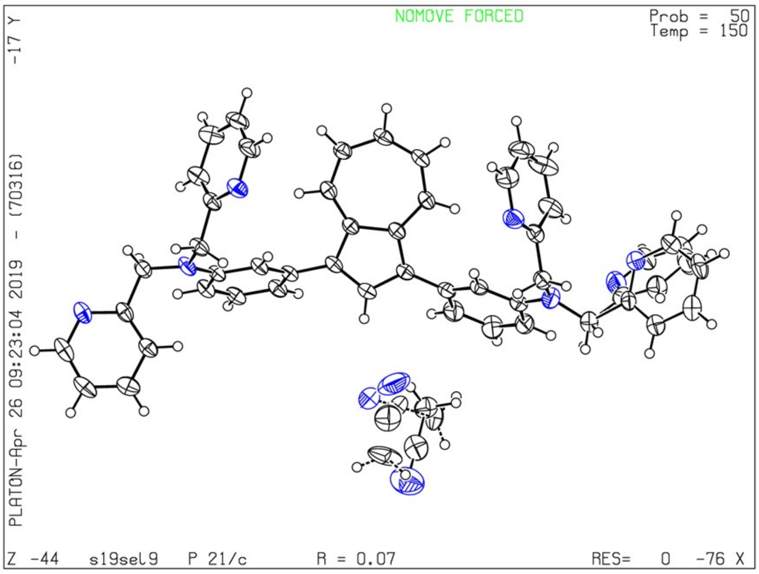
Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1**.

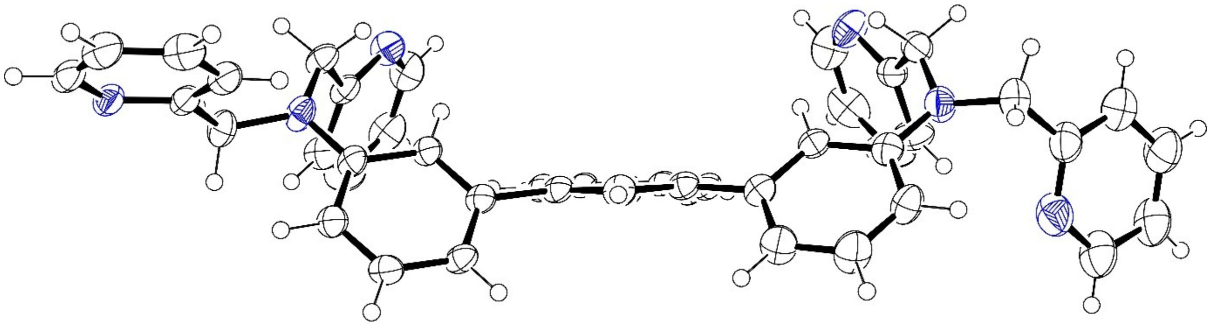
	x	y	z	U(eq)
H(1)	5085	5558	3623	39
H(4)	3130	6248	4899	43
H(5)	2911	4891	5512	49
H(6)	3296	2470	5639	53
H(7)	4059	802	5205	51
H(8)	4868	1249	4580	42
H(12)	2214	6652	4212	42
H(13)	1414	8933	4043	43
H(15)	4057	10806	3684	39
H(16)	4849	8551	3886	38
H(17A)	788	10691	3659	49
H(17B)	863	12521	3608	49
H(19)	-1324	11632	4749	66
H(20)	-387	12321	5357	67
H(21)	1326	12719	5263	72
H(22)	2028	12395	4559	60
H(23A)	3334	12921	3690	45
H(23B)	2303	13722	3565	45
H(25)	1773	11137	2877	77
H(26)	2175	11044	2116	94
H(27)	3604	12341	1871	79
H(28)	4519	13727	2373	85
H(30)	5436	3220	3214	42
H(31)	6628	1790	2850	45
H(33)	7651	207	4028	42
H(34)	6478	1708	4388	41
H(35A)	8971	47	3692	47
H(35B)	9476	-496	3241	47
H(37)	10041	-4742	4055	72
H(38)	8654	-6258	3949	71
H(39)	7281	-5207	3579	64
H(40)	7353	-2640	3333	49
H(41A)	7562	362	2557	53
H(41B)	8517	-728	2591	53
H(43)	10549	2320	1893	77
H(43A)	9574	3331	1779	88
H(44)	10422	4800	2242	82
H(44A)	10709	4424	2292	82
H(45)	9763	4836	2950	72
H(46)	8726	2800	3159	90

Table S7. Torsion angles [°] for **1**.

C(10)-C(1)-C(2)-C(3)	2.19(16)	N(1)-C(23)-C(24)-N(3)	-153.66(15)
C(10)-C(1)-C(2)-C(11)	-176.48(13)	N(1)-C(23)-C(24)-C(25)	29.1(2)
C(1)-C(2)-C(3)-C(4)	170.73(14)	N(3)-C(24)-C(25)-C(26)	-0.4(3)
C(11)-C(2)-C(3)-C(4)	-10.6(2)	C(23)-C(24)-C(25)-C(26)	176.6(2)
C(1)-C(2)-C(3)-C(9)	-3.48(15)	C(24)-C(25)-C(26)-C(27)	1.6(4)
C(11)-C(2)-C(3)-C(9)	175.17(13)	C(25)-C(26)-C(27)-C(28)	-1.3(4)
C(2)-C(3)-C(4)-C(5)	-178.39(15)	C(24)-N(3)-C(28)-C(27)	1.2(4)
C(9)-C(3)-C(4)-C(5)	-5.3(3)	C(26)-C(27)-C(28)-N(3)	-0.1(4)
C(3)-C(4)-C(5)-C(6)	-5.8(3)	C(1)-C(10)-C(29)-C(34)	143.81(14)
C(4)-C(5)-C(6)-C(7)	2.4(3)	C(9)-C(10)-C(29)-C(34)	-37.4(2)
C(5)-C(6)-C(7)-C(8)	7.1(3)	C(1)-C(10)-C(29)-C(30)	-32.2(2)
C(6)-C(7)-C(8)-C(9)	-3.5(3)	C(9)-C(10)-C(29)-C(30)	146.58(14)
C(7)-C(8)-C(9)-C(10)	177.24(15)	C(34)-C(29)-C(30)-C(31)	-1.5(2)
C(7)-C(8)-C(9)-C(3)	-10.5(3)	C(10)-C(29)-C(30)-C(31)	174.89(13)
C(4)-C(3)-C(9)-C(8)	16.0(2)	C(29)-C(30)-C(31)-C(32)	0.3(2)
C(2)-C(3)-C(9)-C(8)	-169.92(14)	C(41)-N(4)-C(32)-C(31)	8.9(2)
C(4)-C(3)-C(9)-C(10)	-170.51(14)	C(35)-N(4)-C(32)-C(31)	165.42(14)
C(2)-C(3)-C(9)-C(10)	3.58(15)	C(41)-N(4)-C(32)-C(33)	-171.11(14)
C(2)-C(1)-C(10)-C(9)	0.12(16)	C(35)-N(4)-C(32)-C(33)	-14.6(2)
C(2)-C(1)-C(10)-C(29)	179.15(13)	C(30)-C(31)-C(32)-N(4)	-178.29(14)
C(8)-C(9)-C(10)-C(1)	171.19(14)	C(30)-C(31)-C(32)-C(33)	1.7(2)
C(3)-C(9)-C(10)-C(1)	-2.25(15)	N(4)-C(32)-C(33)-C(34)	177.33(13)
C(8)-C(9)-C(10)-C(29)	-7.8(2)	C(31)-C(32)-C(33)-C(34)	-2.7(2)
C(3)-C(9)-C(10)-C(29)	178.77(13)	C(32)-C(33)-C(34)-C(29)	1.7(2)
C(1)-C(2)-C(11)-C(16)	-44.2(2)	C(30)-C(29)-C(34)-C(33)	0.5(2)
C(3)-C(2)-C(11)-C(16)	137.37(15)	C(10)-C(29)-C(34)-C(33)	-175.70(13)
C(1)-C(2)-C(11)-C(12)	132.26(16)	C(32)-N(4)-C(35)-C(36)	96.16(16)
C(3)-C(2)-C(11)-C(12)	-46.1(2)	C(41)-N(4)-C(35)-C(36)	-105.94(15)
C(16)-C(11)-C(12)-C(13)	-0.2(2)	C(37)-N(5)-C(36)-C(40)	-0.8(2)
C(2)-C(11)-C(12)-C(13)	-176.85(13)	C(37)-N(5)-C(36)-C(35)	179.18(15)
C(11)-C(12)-C(13)-C(14)	1.1(2)	N(4)-C(35)-C(36)-N(5)	176.68(13)
C(23)-N(1)-C(14)-C(13)	-173.56(14)	N(4)-C(35)-C(36)-C(40)	-3.4(2)
C(17)-N(1)-C(14)-C(13)	-1.7(2)	C(36)-N(5)-C(37)-C(38)	0.3(3)
C(23)-N(1)-C(14)-C(15)	7.1(2)	N(5)-C(37)-C(38)-C(39)	0.3(3)
C(17)-N(1)-C(14)-C(15)	178.97(14)	C(37)-C(38)-C(39)-C(40)	-0.3(3)
C(12)-C(13)-C(14)-N(1)	-179.79(14)	C(38)-C(39)-C(40)-C(36)	-0.1(2)
C(12)-C(13)-C(14)-C(15)	-0.4(2)	N(5)-C(36)-C(40)-C(39)	0.7(2)
N(1)-C(14)-C(15)-C(16)	178.24(13)	C(35)-C(36)-C(40)-C(39)	-179.22(14)
C(13)-C(14)-C(15)-C(16)	-1.1(2)	C(32)-N(4)-C(41)-C(42)	83.40(18)
C(14)-C(15)-C(16)-C(11)	2.1(2)	C(35)-N(4)-C(41)-C(42)	-74.28(17)
C(12)-C(11)-C(16)-C(15)	-1.4(2)	N(4)-C(41)-C(42)-N(6A)	178.8(9)
C(2)-C(11)-C(16)-C(15)	175.25(13)	N(4)-C(41)-C(42)-C(46)	-19.7(3)
C(14)-N(1)-C(17)-C(18)	77.07(19)	N(4)-C(41)-C(42)-N(6)	147.9(4)
C(23)-N(1)-C(17)-C(18)	-110.90(16)	C(44)-C(43)-N(6)-C(42)	-6.6(7)
C(19)-N(2)-C(18)-C(22)	0.7(3)	C(46)-C(42)-N(6)-C(43)	-8.4(5)
C(19)-N(2)-C(18)-C(17)	-178.29(17)	C(41)-C(42)-N(6)-C(43)	-176.2(3)
N(1)-C(17)-C(18)-N(2)	-165.71(15)	C(46)-C(42)-N(6A)-C(43A)	12.1(11)
N(1)-C(17)-C(18)-C(22)	15.3(2)	C(41)-C(42)-N(6A)-C(43A)	174.8(6)
C(18)-N(2)-C(19)-C(20)	-0.5(3)	C(44)-C(43A)-N(6A)-C(42)	15.8(13)
N(2)-C(19)-C(20)-C(21)	0.2(4)	N(6A)-C(43A)-C(44)-C(45)	-34.6(14)
C(19)-C(20)-C(21)-C(22)	0.0(4)	N(6)-C(43)-C(44)-C(45)	17.7(8)
N(2)-C(18)-C(22)-C(21)	-0.5(3)	C(43A)-C(44)-C(45)-C(46)	25.3(9)
C(17)-C(18)-C(22)-C(21)	178.37(19)	C(43)-C(44)-C(45)-C(46)	-12.9(6)
C(20)-C(21)-C(22)-C(18)	0.2(3)	N(6A)-C(42)-C(46)-C(45)	-19.1(9)
C(14)-N(1)-C(23)-C(24)	74.95(18)	N(6)-C(42)-C(46)-C(45)	12.9(5)
C(17)-N(1)-C(23)-C(24)	-97.00(16)	C(41)-C(42)-C(46)-C(45)	179.5(2)
C(28)-N(3)-C(24)-C(25)	-0.9(3)	C(44)-C(45)-C(46)-C(42)	-1.4(4)
C(28)-N(3)-C(24)-C(23)	-178.16(18)		

X-Ray crystallographic data for **2**





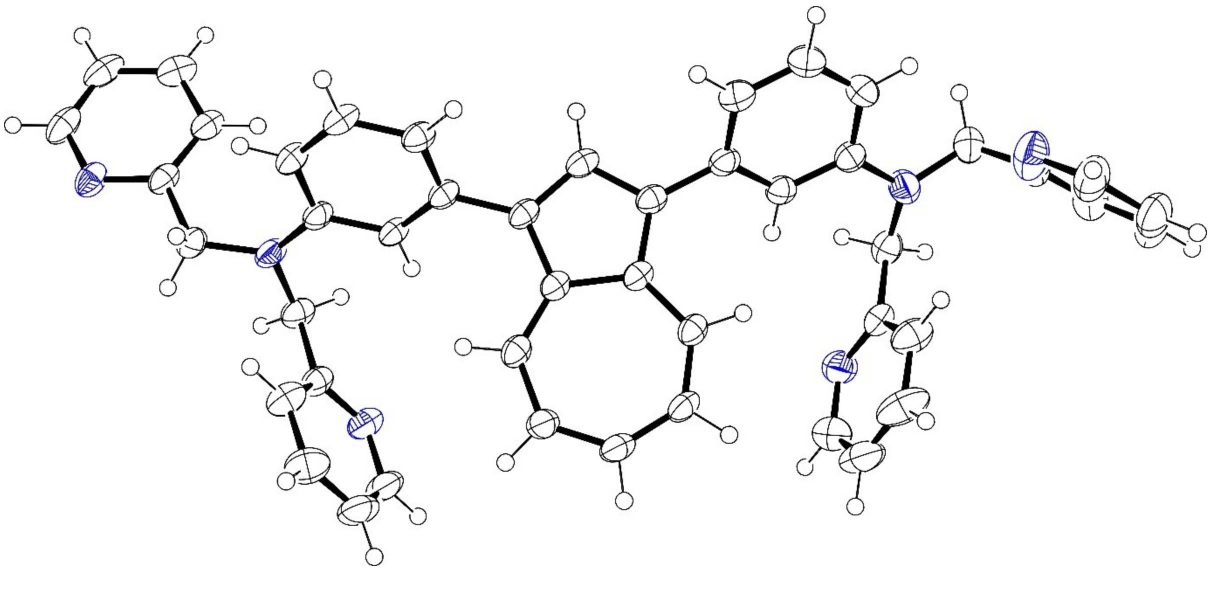


Table S8. Crystal data and structure refinement for **2**.

Identification code	s19sel9	
Empirical formula	$C_{48}H_{41}N_7$	
Formula weight	715.88	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.6047(3) Å	α= 90°.
	b = 9.8218(2) Å	β= 100.398(3)°.
	c = 29.3670(11) Å	γ = 90°.
Volume	3859.65(19) $Å^3$	
Z	4	
Density (calculated)	1.232 Mg/m^3	
Absorption coefficient	0.575 mm^{-1}	
F(000)	1512	
Crystal size	0.336 x 0.172 x 0.055 mm^3	
Theta range for data collection	4.078 to 68.647°.	
Index ranges	-16<=h<=16, -11<=k<=11, -33<=l<=35	
Reflections collected	40045	
Independent reflections	7082 [R(int) = 0.0575]	
Completeness to theta = 67.684°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.68222	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7082 / 18 / 608	
Goodness-of-fit on F^2	1.121	
Final R indices [I>2sigma(I)]	R1 = 0.0688, wR2 = 0.1669	
R indices (all data)	R1 = 0.0880, wR2 = 0.1780	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.364 and -0.222 e.$Å^{-3}$	

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	-279(2)	4345(2)	1758(1)	36(1)
N(2)	1334(2)	7317(3)	1772(1)	42(1)
N(3)	-2870(2)	3487(2)	1226(1)	38(1)
N(4)	6352(2)	4181(3)	4924(1)	42(1)
N(5)	6252(2)	7291(3)	4237(1)	48(1)
C(1)	3174(2)	2598(3)	3257(1)	33(1)
C(2)	2833(2)	3142(3)	2818(1)	29(1)
C(3)	3582(2)	4028(3)	2714(1)	28(1)
C(4)	3568(2)	4698(3)	2300(1)	32(1)
C(5)	4302(2)	5495(3)	2156(1)	34(1)
C(6)	5253(2)	5795(3)	2397(1)	36(1)
C(7)	5719(2)	5403(3)	2835(1)	34(1)
C(8)	5347(2)	4608(3)	3160(1)	31(1)
C(9)	4413(2)	4000(3)	3122(1)	28(1)
C(10)	4115(2)	3122(3)	3451(1)	30(1)
C(11)	1903(2)	2747(3)	2503(1)	30(1)
C(12)	1705(2)	1372(3)	2416(1)	33(1)
C(13)	847(2)	996(3)	2108(1)	34(1)
C(14)	191(2)	1960(3)	1890(1)	34(1)
C(15)	374(2)	3355(3)	1973(1)	31(1)
C(16)	1240(2)	3727(3)	2287(1)	30(1)
C(17)	-19(2)	5773(3)	1817(1)	36(1)
C(18)	845(2)	6210(3)	1585(1)	33(1)
C(19)	1094(2)	5535(3)	1211(1)	45(1)
C(20)	1887(3)	6013(4)	1019(1)	54(1)
C(21)	2397(2)	7148(4)	1207(1)	52(1)
C(22)	2098(2)	7764(3)	1577(1)	48(1)
C(23)	-1111(2)	3975(3)	1394(1)	37(1)
C(24)	-2052(2)	3530(3)	1563(1)	33(1)
C(25)	-2070(2)	3172(3)	2013(1)	36(1)
C(26)	-2969(2)	2768(3)	2132(1)	46(1)
C(27)	-3815(2)	2721(3)	1790(1)	47(1)
C(28)	-3725(2)	3078(3)	1346(1)	43(1)
C(29)	4718(2)	2695(3)	3898(1)	32(1)
C(30)	4798(2)	1316(3)	4006(1)	45(1)
C(31)	5385(3)	900(3)	4414(1)	51(1)
C(32)	5889(2)	1829(3)	4723(1)	43(1)
C(33)	5825(2)	3234(3)	4625(1)	34(1)
C(34)	5223(2)	3638(3)	4210(1)	31(1)
C(35)	6195(2)	5617(3)	4828(1)	38(1)
C(36)	6664(2)	6162(3)	4437(1)	34(1)
C(37)	7472(2)	5541(3)	4297(1)	49(1)
C(38)	7867(3)	6121(4)	3941(2)	63(1)
C(39)	7462(3)	7286(4)	3737(1)	59(1)
C(40)	6656(3)	7836(4)	3895(1)	60(1)
C(41)	6805(2)	3792(4)	5392(1)	47(1)
C(42)	7870(5)	3576(8)	5439(2)	50(2)
C(43)	8535(5)	4426(8)	5706(3)	57(2)
C(44)	9560(5)	4247(9)	5725(3)	64(2)
C(45)	9866(5)	3215(9)	5476(3)	63(2)
C(46)	9146(5)	2360(10)	5209(3)	61(2)
N(6)	8162(4)	2559(7)	5189(2)	60(2)
C(42A)	7735(4)	4640(6)	5607(2)	33(1)
C(43A)	7815(4)	5075(6)	6062(2)	38(1)
C(44A)	8657(5)	5757(6)	6270(2)	45(2)

C(45A)	9389(5)	6022(7)	6013(2)	50(2)
C(46A)	9256(5)	5582(8)	5565(2)	54(2)
N(6A)	8446(4)	4886(6)	5358(2)	49(1)
N(7)	1619(8)	2360(9)	4132(3)	38(2)
C(51)	2166(9)	1797(9)	4381(4)	29(2)
C(52)	2850(20)	1010(30)	4701(8)	42(6)
N(7A)	1332(7)	1086(10)	5006(4)	103(3)
C(51A)	2012(6)	1109(8)	4807(3)	60(2)
C(52A)	2806(12)	1166(16)	4563(4)	49(3)
N(8)	1036(15)	9160(20)	4784(5)	101(6)
C(55)	554(14)	8310(20)	4944(6)	69(4)
C(56)	108(13)	7309(18)	5147(6)	79(6)

Table S10. Bond lengths [Å] for **2**.

N(1)-C(15)	1.389(3)	C(29)-C(30)	1.391(4)
N(1)-C(17)	1.449(4)	C(29)-C(34)	1.395(4)
N(1)-C(23)	1.457(3)	C(30)-C(31)	1.378(4)
N(2)-C(18)	1.339(4)	C(30)-H(30)	0.9500
N(2)-C(22)	1.347(4)	C(31)-C(32)	1.379(5)
N(3)-C(28)	1.337(4)	C(31)-H(31)	0.9500
N(3)-C(24)	1.350(3)	C(32)-C(33)	1.409(4)
N(4)-C(33)	1.386(4)	C(32)-H(32)	0.9500
N(4)-C(35)	1.446(4)	C(32)-H(32A)	0.9500
N(4)-C(41)	1.454(4)	C(33)-C(34)	1.397(4)
N(5)-C(36)	1.331(4)	C(34)-H(34)	0.9500
N(5)-C(40)	1.340(4)	C(35)-C(36)	1.512(4)
C(1)-C(2)	1.395(4)	C(35)-H(35A)	0.9900
C(1)-C(10)	1.402(4)	C(35)-H(35B)	0.9900
C(1)-H(1)	0.9500	C(36)-C(37)	1.383(4)
C(2)-C(3)	1.415(3)	C(37)-C(38)	1.381(5)
C(2)-C(11)	1.478(4)	C(37)-H(37)	0.9500
C(3)-C(4)	1.380(4)	C(38)-C(39)	1.361(6)
C(3)-C(9)	1.492(4)	C(38)-H(38)	0.9500
C(4)-C(5)	1.392(4)	C(39)-C(40)	1.376(5)
C(4)-H(4)	0.9500	C(39)-H(39)	0.9500
C(5)-C(6)	1.389(4)	C(40)-H(40)	0.9500
C(5)-H(5)	0.9500	C(41)-C(42)	1.446(7)
C(6)-C(7)	1.383(4)	C(41)-C(42A)	1.551(6)
C(6)-H(6)	0.9500	C(41)-H(41A)	0.9900
C(7)-C(8)	1.396(4)	C(41)-H(41B)	0.9900
C(7)-H(7)	0.9500	C(41)-H(41C)	0.9900
C(8)-C(9)	1.391(3)	C(41)-H(41D)	0.9900
C(8)-H(8)	0.9500	C(42)-N(6)	1.341(9)
C(9)-C(10)	1.407(4)	C(42)-C(43)	1.370(10)
C(10)-C(29)	1.477(4)	C(43)-C(44)	1.397(10)
C(11)-C(16)	1.392(4)	C(43)-H(43)	0.9500
C(11)-C(12)	1.392(4)	C(44)-C(45)	1.359(12)
C(12)-C(13)	1.391(4)	C(44)-H(44)	0.9500
C(12)-H(12)	0.9500	C(45)-C(46)	1.414(11)
C(13)-C(14)	1.377(4)	C(45)-H(45)	0.9500
C(13)-H(13)	0.9500	C(46)-N(6)	1.343(9)
C(14)-C(15)	1.406(4)	C(46)-H(46)	0.9500
C(14)-H(14)	0.9500	C(42A)-N(6A)	1.337(8)
C(15)-C(16)	1.408(4)	C(42A)-C(43A)	1.388(8)
C(16)-H(16)	0.9500	C(43A)-C(44A)	1.371(8)
C(17)-C(18)	1.522(4)	C(43A)-H(43A)	0.9500
C(17)-H(17A)	0.9900	C(44A)-C(45A)	1.381(10)
C(17)-H(17B)	0.9900	C(44A)-H(44A)	0.9500
C(18)-C(19)	1.378(4)	C(45A)-C(46A)	1.366(10)
C(19)-C(20)	1.387(4)	C(45A)-H(45A)	0.9500
C(19)-H(19)	0.9500	C(46A)-N(6A)	1.344(8)
C(20)-C(21)	1.376(5)	C(46A)-H(46A)	0.9500
C(20)-H(20)	0.9500	N(7)-C(51)	1.094(14)
C(21)-C(22)	1.368(5)	C(51)-C(52)	1.43(2)
C(21)-H(21)	0.9500	C(52)-H(52A)	0.9800
C(22)-H(22)	0.9500	C(52)-H(52B)	0.9800
C(23)-C(24)	1.519(4)	C(52)-H(52C)	0.9800
C(23)-H(23A)	0.9900	N(7A)-C(51A)	1.180(11)
C(23)-H(23B)	0.9900	C(51A)-C(52A)	1.402(16)
C(24)-C(25)	1.371(4)	C(52A)-H(52D)	0.9800
C(25)-C(26)	1.389(4)	C(52A)-H(52E)	0.9800
C(25)-H(25)	0.9500	C(52A)-H(52F)	0.9800
C(26)-C(27)	1.386(5)	N(8)-C(55)	1.20(2)
C(26)-H(26)	0.9500	C(55)-C(56)	1.35(2)
C(27)-C(28)	1.377(5)	C(56)-H(56A)	0.9800
C(27)-H(27)	0.9500	C(56)-H(56B)	0.9800
C(28)-H(28)	0.9500	C(56)-H(56C)	0.9800

Table S11. Bond angles [°] for **2**.

C(15)-N(1)-C(17)	120.0(2)	N(1)-C(17)-H(17A)	108.7
C(15)-N(1)-C(23)	120.5(2)	C(18)-C(17)-H(17A)	108.7
C(17)-N(1)-C(23)	118.1(2)	N(1)-C(17)-H(17B)	108.7
C(18)-N(2)-C(22)	117.2(3)	C(18)-C(17)-H(17B)	108.7
C(28)-N(3)-C(24)	117.2(3)	H(17A)-C(17)-H(17B)	107.6
C(33)-N(4)-C(35)	119.4(2)	N(2)-C(18)-C(19)	122.7(3)
C(33)-N(4)-C(41)	120.3(3)	N(2)-C(18)-C(17)	114.4(3)
C(35)-N(4)-C(41)	117.5(3)	C(19)-C(18)-C(17)	122.8(3)
C(36)-N(5)-C(40)	117.8(3)	C(18)-C(19)-C(20)	118.9(3)
C(2)-C(1)-C(10)	111.2(2)	C(18)-C(19)-H(19)	120.6
C(2)-C(1)-H(1)	124.4	C(20)-C(19)-H(19)	120.6
C(10)-C(1)-H(1)	124.4	C(21)-C(20)-C(19)	118.9(3)
C(1)-C(2)-C(3)	107.7(2)	C(21)-C(20)-H(20)	120.6
C(1)-C(2)-C(11)	125.6(2)	C(19)-C(20)-H(20)	120.6
C(3)-C(2)-C(11)	126.5(2)	C(22)-C(21)-C(20)	118.6(3)
C(4)-C(3)-C(2)	126.0(2)	C(22)-C(21)-H(21)	120.7
C(4)-C(3)-C(9)	127.2(2)	C(20)-C(21)-H(21)	120.7
C(2)-C(3)-C(9)	106.6(2)	N(2)-C(22)-C(21)	123.7(3)
C(3)-C(4)-C(5)	129.7(3)	N(2)-C(22)-H(22)	118.1
C(3)-C(4)-H(4)	115.1	C(21)-C(22)-H(22)	118.1
C(5)-C(4)-H(4)	115.1	N(1)-C(23)-C(24)	114.8(2)
C(6)-C(5)-C(4)	128.1(3)	N(1)-C(23)-H(23A)	108.6
C(6)-C(5)-H(5)	115.9	C(24)-C(23)-H(23A)	108.6
C(4)-C(5)-H(5)	115.9	N(1)-C(23)-H(23B)	108.6
C(7)-C(6)-C(5)	130.0(3)	C(24)-C(23)-H(23B)	108.6
C(7)-C(6)-H(6)	115.0	H(23A)-C(23)-H(23B)	107.5
C(5)-C(6)-H(6)	115.0	N(3)-C(24)-C(25)	122.8(3)
C(6)-C(7)-C(8)	129.0(2)	N(3)-C(24)-C(23)	113.6(3)
C(6)-C(7)-H(7)	115.5	C(25)-C(24)-C(23)	123.5(2)
C(8)-C(7)-H(7)	115.5	C(24)-C(25)-C(26)	119.1(3)
C(9)-C(8)-C(7)	128.7(3)	C(24)-C(25)-H(25)	120.5
C(9)-C(8)-H(8)	115.7	C(26)-C(25)-H(25)	120.5
C(7)-C(8)-H(8)	115.7	C(27)-C(26)-C(25)	118.8(3)
C(8)-C(9)-C(10)	125.5(2)	C(27)-C(26)-H(26)	120.6
C(8)-C(9)-C(3)	127.2(2)	C(25)-C(26)-H(26)	120.6
C(10)-C(9)-C(3)	107.0(2)	C(28)-C(27)-C(26)	118.3(3)
C(1)-C(10)-C(9)	107.5(2)	C(28)-C(27)-H(27)	120.9
C(1)-C(10)-C(29)	125.2(2)	C(26)-C(27)-H(27)	120.9
C(9)-C(10)-C(29)	126.9(2)	N(3)-C(28)-C(27)	123.8(3)
C(16)-C(11)-C(12)	119.9(2)	N(3)-C(28)-H(28)	118.1
C(16)-C(11)-C(2)	121.0(2)	C(27)-C(28)-H(28)	118.1
C(12)-C(11)-C(2)	119.1(2)	C(30)-C(29)-C(34)	119.2(3)
C(13)-C(12)-C(11)	119.3(3)	C(30)-C(29)-C(10)	119.2(3)
C(13)-C(12)-H(12)	120.3	C(34)-C(29)-C(10)	121.7(2)
C(11)-C(12)-H(12)	120.3	C(31)-C(30)-C(29)	119.8(3)
C(14)-C(13)-C(12)	121.1(3)	C(31)-C(30)-H(30)	120.1
C(14)-C(13)-H(13)	119.5	C(29)-C(30)-H(30)	120.1
C(12)-C(13)-H(13)	119.5	C(30)-C(31)-C(32)	121.2(3)
C(13)-C(14)-C(15)	120.7(2)	C(30)-C(31)-H(31)	119.4
C(13)-C(14)-H(14)	119.7	C(32)-C(31)-H(31)	119.4
C(15)-C(14)-H(14)	119.7	C(31)-C(32)-C(33)	120.6(3)
N(1)-C(15)-C(14)	121.7(2)	C(31)-C(32)-H(32)	119.7
N(1)-C(15)-C(16)	120.4(2)	C(33)-C(32)-H(32)	119.7
C(14)-C(15)-C(16)	117.9(2)	C(31)-C(32)-H(32A)	119.7
C(11)-C(16)-C(15)	121.1(2)	C(33)-C(32)-H(32A)	119.7
C(11)-C(16)-H(16)	119.5	N(4)-C(33)-C(34)	121.1(3)
C(15)-C(16)-H(16)	119.5	N(4)-C(33)-C(32)	121.5(3)
N(1)-C(17)-C(18)	114.3(2)	C(34)-C(33)-C(32)	117.5(3)

C(29)-C(34)-C(33)	121.8(3)	C(44)-C(45)-C(46)	119.5(7)
C(29)-C(34)-H(34)	119.1	C(44)-C(45)-H(45)	120.2
C(33)-C(34)-H(34)	119.1	C(46)-C(45)-H(45)	120.2
N(4)-C(35)-C(36)	115.1(2)	N(6)-C(46)-C(45)	121.5(8)
N(4)-C(35)-H(35A)	108.5	N(6)-C(46)-H(46)	119.3
C(36)-C(35)-H(35A)	108.5	C(45)-C(46)-H(46)	119.3
N(4)-C(35)-H(35B)	108.5	C(42)-N(6)-C(46)	118.4(7)
C(36)-C(35)-H(35B)	108.5	N(6A)-C(42A)-C(43A)	122.3(5)
H(35A)-C(35)-H(35B)	107.5	N(6A)-C(42A)-C(41)	119.4(5)
N(5)-C(36)-C(37)	122.1(3)	C(43A)-C(42A)-C(41)	118.3(5)
N(5)-C(36)-C(35)	115.4(2)	C(44A)-C(43A)-C(42A)	119.6(6)
C(37)-C(36)-C(35)	122.6(3)	C(44A)-C(43A)-H(43A)	120.2
C(38)-C(37)-C(36)	118.8(3)	C(42A)-C(43A)-H(43A)	120.2
C(38)-C(37)-H(37)	120.6	C(43A)-C(44A)-C(45A)	118.4(6)
C(36)-C(37)-H(37)	120.6	C(43A)-C(44A)-H(44A)	120.8
C(39)-C(38)-C(37)	119.8(3)	C(45A)-C(44A)-H(44A)	120.8
C(39)-C(38)-H(38)	120.1	C(46A)-C(45A)-C(44A)	119.0(6)
C(37)-C(38)-H(38)	120.1	C(46A)-C(45A)-H(45A)	120.5
C(38)-C(39)-C(40)	117.8(3)	C(44A)-C(45A)-H(45A)	120.5
C(38)-C(39)-H(39)	121.1	N(6A)-C(46A)-C(45A)	123.5(6)
C(40)-C(39)-H(39)	121.1	N(6A)-C(46A)-H(46A)	118.3
N(5)-C(40)-C(39)	123.7(4)	C(45A)-C(46A)-H(46A)	118.3
N(5)-C(40)-H(40)	118.1	C(42A)-N(6A)-C(46A)	117.3(6)
C(39)-C(40)-H(40)	118.1	N(7)-C(51)-C(52)	177.4(17)
C(42)-C(41)-N(4)	111.9(4)	C(51)-C(52)-H(52A)	109.5
N(4)-C(41)-C(42A)	114.8(3)	C(51)-C(52)-H(52B)	109.5
C(42)-C(41)-H(41A)	109.2	H(52A)-C(52)-H(52B)	109.5
N(4)-C(41)-H(41A)	109.2	C(51)-C(52)-H(52C)	109.5
C(42)-C(41)-H(41B)	109.2	H(52A)-C(52)-H(52C)	109.5
N(4)-C(41)-H(41B)	109.2	H(52B)-C(52)-H(52C)	109.5
H(41A)-C(41)-H(41B)	107.9	N(7A)-C(51A)-C(52A)	178.4(11)
N(4)-C(41)-H(41C)	108.6	C(51A)-C(52A)-H(52D)	109.5
C(42A)-C(41)-H(41C)	108.6	C(51A)-C(52A)-H(52E)	109.5
N(4)-C(41)-H(41D)	108.6	H(52D)-C(52A)-H(52E)	109.5
C(42A)-C(41)-H(41D)	108.6	C(51A)-C(52A)-H(52F)	109.5
H(41C)-C(41)-H(41D)	107.5	H(52D)-C(52A)-H(52F)	109.5
N(6)-C(42)-C(43)	122.5(7)	H(52E)-C(52A)-H(52F)	109.5
N(6)-C(42)-C(41)	116.7(6)	N(8)-C(55)-C(56)	174(2)
C(43)-C(42)-C(41)	120.8(7)	C(55)-C(56)-H(56A)	109.5
C(42)-C(43)-C(44)	119.8(8)	C(55)-C(56)-H(56B)	109.5
C(42)-C(43)-H(43)	120.1	H(56A)-C(56)-H(56B)	109.5
C(44)-C(43)-H(43)	120.1	C(55)-C(56)-H(56C)	109.5
C(45)-C(44)-C(43)	118.2(7)	H(56A)-C(56)-H(56C)	109.5
C(45)-C(44)-H(44)	120.9	H(56B)-C(56)-H(56C)	109.5
C(43)-C(44)-H(44)	120.9		

Table S12. Anisotropic displacement parameters ($Å^2$x 10^3) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	22(1)	32(1)	54(2)	6(1)	3(1)	-6(1)
N(2)	35(1)	36(1)	56(2)	1(1)	10(1)	-7(1)
N(3)	25(1)	32(1)	54(2)	-4(1)	3(1)	1(1)
N(4)	45(1)	40(1)	37(1)	2(1)	-1(1)	0(1)
N(5)	36(1)	50(2)	57(2)	13(1)	11(1)	4(1)
C(1)	26(1)	33(1)	42(2)	0(1)	11(1)	-5(1)
C(2)	21(1)	27(1)	41(2)	-3(1)	9(1)	-1(1)
C(3)	22(1)	24(1)	38(1)	-1(1)	7(1)	2(1)
C(4)	23(1)	30(1)	41(2)	-2(1)	5(1)	2(1)
C(5)	30(1)	32(1)	42(2)	5(1)	7(1)	-2(1)
C(6)	29(1)	32(1)	50(2)	4(1)	12(1)	-6(1)
C(7)	21(1)	33(1)	49(2)	0(1)	8(1)	-5(1)
C(8)	23(1)	28(1)	41(2)	-2(1)	4(1)	1(1)
C(9)	22(1)	24(1)	39(2)	-2(1)	8(1)	2(1)
C(10)	25(1)	29(1)	38(2)	0(1)	9(1)	0(1)
C(11)	21(1)	32(1)	37(2)	-2(1)	9(1)	-3(1)
C(12)	24(1)	27(1)	47(2)	1(1)	9(1)	1(1)
C(13)	28(1)	27(1)	50(2)	-6(1)	13(1)	-6(1)
C(14)	24(1)	34(1)	45(2)	-4(1)	7(1)	-5(1)
C(15)	20(1)	33(1)	40(2)	2(1)	8(1)	-4(1)
C(16)	22(1)	27(1)	41(2)	-2(1)	7(1)	-4(1)
C(17)	24(1)	34(2)	52(2)	4(1)	11(1)	2(1)
C(18)	23(1)	28(1)	49(2)	4(1)	6(1)	1(1)
C(19)	37(2)	42(2)	59(2)	-3(1)	16(1)	-6(1)
C(20)	50(2)	55(2)	62(2)	1(2)	27(2)	-3(2)
C(21)	35(2)	53(2)	70(2)	17(2)	17(2)	-8(1)
C(22)	38(2)	43(2)	64(2)	7(2)	9(2)	-15(1)
C(23)	24(1)	41(2)	45(2)	6(1)	3(1)	-5(1)
C(24)	23(1)	24(1)	50(2)	-1(1)	3(1)	1(1)
C(25)	28(1)	29(1)	52(2)	0(1)	8(1)	-3(1)
C(26)	44(2)	37(2)	60(2)	0(1)	19(2)	-5(1)
C(27)	29(2)	36(2)	80(2)	-6(2)	16(2)	-8(1)
C(28)	23(1)	31(2)	72(2)	-9(1)	3(1)	-1(1)
C(29)	26(1)	33(1)	39(2)	3(1)	9(1)	-3(1)
C(30)	47(2)	33(2)	54(2)	4(1)	3(2)	-9(1)
C(31)	56(2)	33(2)	61(2)	12(2)	-2(2)	-6(1)
C(32)	39(2)	40(2)	48(2)	14(1)	1(1)	2(1)
C(33)	28(1)	40(2)	36(2)	2(1)	9(1)	-1(1)
C(34)	26(1)	31(1)	37(2)	3(1)	10(1)	1(1)
C(35)	33(1)	44(2)	37(2)	-6(1)	7(1)	-2(1)
C(36)	28(1)	34(1)	40(2)	-6(1)	5(1)	-5(1)
C(37)	41(2)	39(2)	69(2)	-5(2)	22(2)	-1(1)
C(38)	60(2)	55(2)	86(3)	-19(2)	45(2)	-18(2)
C(39)	66(2)	60(2)	56(2)	-4(2)	25(2)	-28(2)
C(40)	56(2)	59(2)	63(2)	18(2)	9(2)	-7(2)
C(41)	39(2)	57(2)	41(2)	5(2)	-2(1)	-5(2)
C(42)	45(4)	65(5)	38(3)	6(3)	4(3)	4(3)
C(43)	48(4)	64(5)	57(5)	5(4)	1(3)	0(3)
C(44)	41(4)	74(5)	73(5)	-1(4)	-3(3)	-7(4)
C(45)	32(3)	95(6)	60(5)	6(4)	8(3)	-7(4)
C(46)	35(4)	89(6)	60(5)	2(4)	7(3)	-5(4)
N(6)	38(3)	88(5)	53(4)	-10(3)	6(3)	0(3)
C(42A)	29(3)	29(3)	37(3)	4(2)	-4(2)	-2(2)
C(43A)	37(3)	33(3)	44(3)	-1(2)	3(3)	2(2)
C(44A)	45(3)	35(3)	50(4)	-9(3)	-4(3)	8(3)

C(45A)	37(3)	43(4)	64(4)	-5(3)	-10(3)	-11(3)
C(46A)	41(3)	67(5)	54(4)	6(3)	5(3)	-20(3)
N(6A)	43(3)	67(4)	37(3)	2(3)	3(2)	-18(3)
N(7)	53(6)	22(4)	39(5)	-8(4)	9(5)	7(4)
C(51)	52(7)	7(4)	28(5)	-7(4)	5(5)	10(5)
C(52)	47(8)	32(7)	43(10)	0(8)	-7(7)	14(6)
N(7A)	85(6)	101(7)	131(8)	22(6)	40(6)	12(5)
C(51A)	59(5)	49(4)	71(5)	1(4)	7(4)	3(3)
C(52A)	64(6)	43(6)	42(6)	-12(5)	15(5)	-7(5)
N(8)	131(15)	129(16)	50(9)	8(9)	36(9)	-25(13)
C(55)	72(6)	74(6)	64(6)	-13(5)	19(5)	9(5)
C(56)	88(12)	83(12)	85(12)	-49(10)	67(10)	-42(10)

Table S13. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **2**.

	x	y	z	U(eq)
H(1)	2814	1957	3405	40
H(4)	2968	4602	2080	38
H(5)	4131	5881	1856	41
H(6)	5643	6358	2236	44
H(7)	6385	5719	2929	41
H(8)	5792	4462	3444	37
H(12)	2151	698	2564	39
H(13)	711	58	2048	41
H(14)	-391	1679	1682	41
H(16)	1375	4663	2352	36
H(17A)	159	5971	2153	43
H(17B)	-613	6326	1690	43
H(19)	728	4755	1086	54
H(20)	2075	5564	761	64
H(21)	2945	7497	1083	62
H(22)	2450	8552	1704	58
H(23A)	-894	3226	1209	45
H(23B)	-1276	4766	1185	45
H(25)	-1476	3200	2240	43
H(26)	-3002	2528	2442	55
H(27)	-4442	2450	1860	57
H(28)	-4304	3030	1111	52
H(30)	4450	663	3798	55
H(31)	5443	-44	4485	62
H(32)	6282	1520	5005	52
H(32A)	6282	1520	5005	52
H(34)	5156	4581	4139	37
H(35A)	6465	6134	5113	45
H(35B)	5466	5790	4755	45
H(37)	7751	4731	4443	58
H(38)	8420	5708	3839	76
H(39)	7727	7705	3494	71
H(40)	6370	8649	3754	71
H(41A)	6681	4516	5610	56
H(41B)	6487	2945	5477	56
H(41C)	7001	2821	5391	56
H(41D)	6296	3878	5593	56
H(43)	8300	5134	5879	69
H(44)	10031	4833	5907	77
H(45)	10558	3068	5481	75
H(46)	9363	1629	5040	74
H(43A)	7290	4901	6228	46
H(44A)	8733	6041	6584	54
H(45A)	9977	6504	6145	61
H(46A)	9763	5777	5390	65
H(52A)	2637	1000	5002	64
H(52B)	3521	1411	4735	64
H(52C)	2869	75	4585	64
H(52D)	2684	1895	4332	73
H(52E)	2860	294	4408	73
H(52F)	3430	1350	4779	73
H(56A)	-604	7275	5011	119
H(56B)	184	7490	5480	119
H(56C)	421	6436	5099	119

Table S14. Torsion angles [°] for **2**.

C(10)-C(1)-C(2)-C(3)	1.3(3)	N(3)-C(24)-C(25)-C(26)	-1.2(4)
C(10)-C(1)-C(2)-C(11)	175.7(2)	C(23)-C(24)-C(25)-C(26)	-179.5(3)
C(1)-C(2)-C(3)-C(4)	175.3(3)	C(24)-C(25)-C(26)-C(27)	1.0(4)
C(11)-C(2)-C(3)-C(4)	1.0(4)	C(25)-C(26)-C(27)-C(28)	0.0(5)
C(1)-C(2)-C(3)-C(9)	-0.3(3)	C(24)-N(3)-C(28)-C(27)	0.8(4)
C(11)-C(2)-C(3)-C(9)	-174.5(2)	C(26)-C(27)-C(28)-N(3)	-1.0(5)
C(2)-C(3)-C(4)-C(5)	-174.3(3)	C(1)-C(10)-C(29)-C(30)	43.5(4)
C(9)-C(3)-C(4)-C(5)	0.4(5)	C(9)-C(10)-C(29)-C(30)	-129.1(3)
C(3)-C(4)-C(5)-C(6)	1.2(5)	C(1)-C(10)-C(29)-C(34)	-137.6(3)
C(4)-C(5)-C(6)-C(7)	-0.4(5)	C(9)-C(10)-C(29)-C(34)	49.8(4)
C(5)-C(6)-C(7)-C(8)	-1.2(5)	C(34)-C(29)-C(30)-C(31)	-1.0(5)
C(6)-C(7)-C(8)-C(9)	0.5(5)	C(10)-C(29)-C(30)-C(31)	177.9(3)
C(7)-C(8)-C(9)-C(10)	174.8(3)	C(29)-C(30)-C(31)-C(32)	0.7(5)
C(7)-C(8)-C(9)-C(3)	1.7(5)	C(30)-C(31)-C(32)-C(33)	-0.8(5)
C(4)-C(3)-C(9)-C(8)	-2.3(4)	C(35)-N(4)-C(33)-C(34)	6.5(4)
C(2)-C(3)-C(9)-C(8)	173.2(2)	C(41)-N(4)-C(33)-C(34)	167.2(3)
C(4)-C(3)-C(9)-C(10)	-176.4(3)	C(35)-N(4)-C(33)-C(32)	-174.5(3)
C(2)-C(3)-C(9)-C(10)	-0.9(3)	C(41)-N(4)-C(33)-C(32)	-13.9(4)
C(2)-C(1)-C(10)-C(9)	-1.9(3)	C(31)-C(32)-C(33)-N(4)	-177.9(3)
C(2)-C(1)-C(10)-C(29)	-175.7(2)	C(31)-C(32)-C(33)-C(34)	1.1(4)
C(8)-C(9)-C(10)-C(1)	-172.5(3)	C(30)-C(29)-C(34)-C(33)	1.4(4)
C(3)-C(9)-C(10)-C(1)	1.7(3)	C(10)-C(29)-C(34)-C(33)	-177.5(2)
C(8)-C(9)-C(10)-C(29)	1.1(4)	N(4)-C(33)-C(34)-C(29)	177.5(3)
C(3)-C(9)-C(10)-C(29)	175.4(2)	C(32)-C(33)-C(34)-C(29)	-1.5(4)
C(1)-C(2)-C(11)-C(16)	132.0(3)	C(33)-N(4)-C(35)-C(36)	-74.5(3)
C(3)-C(2)-C(11)-C(16)	-54.7(4)	C(41)-N(4)-C(35)-C(36)	124.3(3)
C(1)-C(2)-C(11)-C(12)	-49.4(4)	C(40)-N(5)-C(36)-C(37)	-1.0(5)
C(3)-C(2)-C(11)-C(12)	123.8(3)	C(40)-N(5)-C(36)-C(35)	178.4(3)
C(16)-C(11)-C(12)-C(13)	0.6(4)	N(4)-C(35)-C(36)-N(5)	156.9(3)
C(2)-C(11)-C(12)-C(13)	-178.0(2)	N(4)-C(35)-C(36)-C(37)	-23.7(4)
C(11)-C(12)-C(13)-C(14)	-0.1(4)	N(5)-C(36)-C(37)-C(38)	0.5(5)
C(12)-C(13)-C(14)-C(15)	0.1(4)	C(35)-C(36)-C(37)-C(38)	-178.8(3)
C(17)-N(1)-C(15)-C(14)	-174.1(3)	C(36)-C(37)-C(38)-C(39)	0.3(5)
C(23)-N(1)-C(15)-C(14)	-8.0(4)	C(37)-C(38)-C(39)-C(40)	-0.6(6)
C(17)-N(1)-C(15)-C(16)	6.7(4)	C(36)-N(5)-C(40)-C(39)	0.7(5)
C(23)-N(1)-C(15)-C(16)	172.8(2)	C(38)-C(39)-C(40)-N(5)	0.1(6)
C(13)-C(14)-C(15)-N(1)	-179.7(3)	C(33)-N(4)-C(41)-C(42)	102.1(4)
C(13)-C(14)-C(15)-C(16)	-0.5(4)	C(35)-N(4)-C(41)-C(42)	-96.9(5)
C(12)-C(11)-C(16)-C(15)	-1.1(4)	C(33)-N(4)-C(41)-C(42A)	152.8(3)
C(2)-C(11)-C(16)-C(15)	177.5(2)	C(35)-N(4)-C(41)-C(42A)	-46.2(4)
N(1)-C(15)-C(16)-C(11)	-179.8(2)	N(4)-C(41)-C(42)-N(6)	-63.3(7)
C(14)-C(15)-C(16)-C(11)	1.0(4)	N(4)-C(41)-C(42)-C(43)	113.3(6)
C(15)-N(1)-C(17)-C(18)	68.7(3)	N(6)-C(42)-C(43)-C(44)	0.2(12)
C(23)-N(1)-C(17)-C(18)	-97.7(3)	C(41)-C(42)-C(43)-C(44)	-176.3(6)
C(22)-N(2)-C(18)-C(19)	-0.1(4)	C(42)-C(43)-C(44)-C(45)	-0.6(12)
C(22)-N(2)-C(18)-C(17)	-179.2(3)	C(43)-C(44)-C(45)-C(46)	-0.1(12)
N(1)-C(17)-C(18)-N(2)	-155.9(2)	C(44)-C(45)-C(46)-N(6)	1.2(13)
N(1)-C(17)-C(18)-C(19)	25.0(4)	C(43)-C(42)-N(6)-C(46)	0.8(11)
N(2)-C(18)-C(19)-C(20)	0.4(5)	C(41)-C(42)-N(6)-C(46)	177.5(6)
C(17)-C(18)-C(19)-C(20)	179.4(3)	C(45)-C(46)-N(6)-C(42)	-1.5(12)
C(18)-C(19)-C(20)-C(21)	-0.2(5)	N(4)-C(41)-C(42A)-N(6A)	-46.1(6)
C(19)-C(20)-C(21)-C(22)	-0.2(5)	N(4)-C(41)-C(42A)-C(43A)	136.3(4)
C(18)-N(2)-C(22)-C(21)	-0.4(5)	N(6A)-C(42A)-C(43A)-C(44A)	-1.4(9)
C(20)-C(21)-C(22)-N(2)	0.5(5)	C(41)-C(42A)-C(43A)-C(44A)	176.2(5)
C(15)-N(1)-C(23)-C(24)	85.9(3)	C(42A)-C(43A)-C(44A)-C(45A)	1.8(9)
C(17)-N(1)-C(23)-C(24)	-107.7(3)	C(43A)-C(44A)-C(45A)-C(46A)	-0.9(10)
C(28)-N(3)-C(24)-C(25)	0.3(4)	C(44A)-C(45A)-C(46A)-N(6A)	-0.5(11)
C(28)-N(3)-C(24)-C(23)	178.7(2)	C(43A)-C(42A)-N(6A)-C(46A)	0.0(9)
N(1)-C(23)-C(24)-N(3)	166.0(2)	C(41)-C(42A)-N(6A)-C(46A)	-177.6(5)
N(1)-C(23)-C(24)-C(25)	-15.5(4)	C(45A)-C(46A)-N(6A)-C(42A)	1.0(11)

References

1. V. V. Kouznetsov, L. Y. Vargas Méndez, M. Sortino, Y. Vásquez, M. P. Gupta, M. Freile, R. D. Enriz and S. A. Zacchino, *Bioorg. Med. Chem.*, 2008, **16**, 794–809.
2. Y. Wang, H. Liu, X. Zhang, Z. Zhang and D. Huang, *Org. Biomol. Chem.*, 2017, **15**, 9164–9168.
3. S. Son and K. Yamada, *Bull. Chem. Soc. Jpn.*, 2013, **86**, 37–44.
4. M. Macias-Contreras, K. L. Daykin, J. T. Simmons, J. R. Allen, Z. S. Hooper, W. Davidson and L. Zhu, *Org. Biomol. Chem.*, 2017, **15**, 9139–9148.
5. C. Gwizdala, D. P. Kennedy, and S. C. Burdette, *Chem. Commun.*, 2009, 6967–6969.
6. C. Gwizdala, C. V. Singh, T. R. Friss, J. C. MacDonald, and S. C. Burdette, *Dalton Trans.*, 2012, **41**, 8162–8174.
7. H. Salman, Y. Abraham, S. Tal, S. Meltzman, M. Kapon, N. Tessler, S. Speiser and Y. Eichen, *Eur. J. Org. Chem.*, 2005, 2207–2212.