# Supporting information

## Synthesis and photophysical properties about the biaryl systems of pyrrocytidine and furouridine with benzothiophene, benzofuran, and benzene as the aromatic extended moiety

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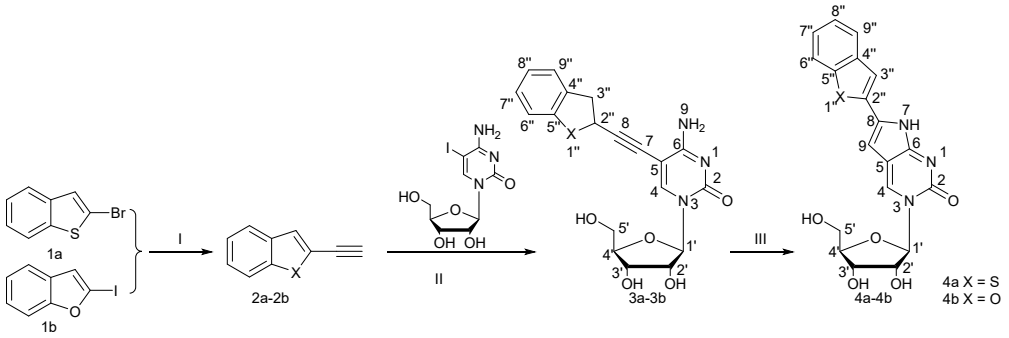
## 1. General information

### *1.1. General information of materiel and instrument*

All reagents were purchased from commercial sources and used without further purification, unless otherwise noted. Triethylamine and *N*,*N*-dimethylformamide were freshly distilled over $CaH_2$. Moister and oxygen sensitive reactions were performed in an inert nitrogen atmosphere. Aqueous samples were prepared with deionized water. For all spectroscopic measurements, a 1 cm four-sided Helma quartz cuvette was used. All spectroscopy samples were prepared from concentrated DMSO stock solutions. Hence, all samples contain 0.4 v% DMSO. NMR spectra were recorded at 25 °C on a Bruker Avance III HD 400 MHz spectrometer. Mass spectra were recorded at Waters MaldiSynapt instrument. Absorption spectra were measured on a Persee TU-1901, UV-Vis spectrophotometer and corrected for the blank. The sample temperature was kept constant at 25 °C using a thermostat. Steady state emission and excitation spectra were taken on a CARY Eclipse luminescence spectrometer with a 1 nm resolution. Time-resolved fluorescence spectra were measured by FLS-920 steady-state spectroscopy using a standard time-correlated and single-photon counting scheme.

### *1.2. General procedure for formation of 4a-4b.*




*1.2.1 Synthesis of 2-ethynylbenzo[b]thiophene (**2a**)*

Successively add 2-bromobenzothiophene (150.0 mg, 0.7 mmol), bis(triphenylphosphine) palladium dichloride (12.0 mg, 0.025 mmol) and cuprous iodide (CuI) (12.0 mg, 0.09 mmol) into a 10 mL reaction flask, vacuumize and fill with nitrogen for protection, then add anhydrous triethylamine (2.0 mL) as solvent, stir at 70 ºC for half an hour to fully react, *N*-(trimethylsilyl)acetamide (TMSA) (171.8 mg, 1.8 mmol) was added until the reaction was complete. After the reaction was stopped, the reaction solution was diluted with ethyl acetate, and the catalyst was removed by diatomite filtration; The filtrate was spin dried and separated by column chromatography to obtain the intermediate product (2-ethynylbenzothiophene) trimethylsilane. (2-ethynylbenzothiophene) trimethylsilane (230.4 mg, 1.0 mmol), potassium carbonate (414.6 mg, 3.0 mmol) and methanol (10.0 mL) were successively added into a 25 mL reaction flask and stirred at room temperature for about 2 hours until the reaction was complete. After the reaction was stopped, the reaction solution was diluted with dichloromethane, extracted with saturated NaCl aqueous solution, and the organic layer was dried with anhydrous $MgSO_4$; The liquid was spin dried and separated by column chromatography (the eluent was petroleum ether: ethyl acetate = 10: 1) to afford compound **2a** (83 mg, 75%) as dark brown viscous liquid.

*1.2.2 Synthesis of 2-ethynylbenzofuran (**2b**)*

Benzofuran-2-boric acid (160.0 mg, 1.000 mmol), *N*-iodo succinimide (NIS) (225.0 mg, 1.000 mmol) and anhydrous acetonitrile (5.0 mL) were added to a 10 mL reaction flask, protected with

nitrogen, and reacted at room temperature without light for about 24 hours until the reaction was complete. After the reaction stopped, the intermediate product 2-iodobenzofuran was separated by column chromatography. Under the protection of nitrogen, 2-iodobenzofuran (244.0 mg, 1.000 mmol), bis (triphenylphosphine) palladium dichloride (17.5 mg, 0.025 mmol) and cuprous iodide (CuI) (17.1 mg, 0.090 mmol) were successively added to 10 mL reaction tube. Vacuumize and fill with nitrogen for protection, then add anhydrous triethylamine (4.0 mL) as solvent, stir at 70 °C for half an hour to fully react, add trimethylethynyl silicon (TMSA) (245.5 mg, 2.500 mmol), and continue the reaction for about 12 hours until the reaction is complete (TLC plate monitors the reaction, and the developing agent is petroleum ether). After the reaction was stopped, the reaction solution was diluted with ethyl acetate, and the catalyst was removed by diatomite filtration; The filtrate was spin dried and separated by column chromatography to obtain the intermediate product (2-ethynylbenzofuran) trimethylsilane. (2-ethynylbenzofuran) trimethylsilane (214.3 mg, 1.000 mmol), potassium carbonate (414.6 mg, 3.000 mmol) and methanol (10.0 mL) were successively added to a 25 mL reaction flask and stirred at room temperature for about 2 hours until the reaction was complete; Add dichloromethane to dilute the reaction solution, extract with saturated NaCl aqueous solution, and dry the organic layer with anhydrous $MgSO_4$; The liquid was spin dried and separated by column chromatography (the eluent was petroleum ether: ethyl acetate = 10: 1) to afford compound **2b** (97 mg, 68%) as dark brown viscous liquid.

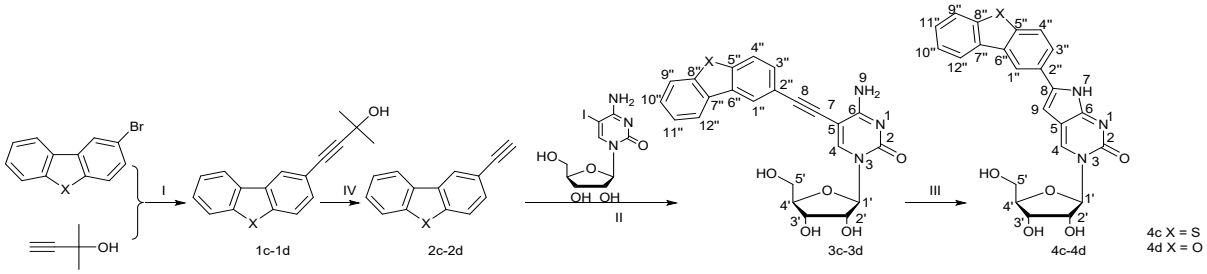
*1.2.3 Synthesis of 5-benzoheterocyclic ethynyl cytidine (**3a-3b**)*

Add 5-iodocarcidine (185 mg, 0.500 mmol), [1,1'-bis(diphenylphosphino)ferrocene] palladium dichloride (19.0 mg, 0.030 mmol) and cuprous iodide (CuI) (3.5 mg, 0.020 mmol) into a 25 mL reaction flask, anhydrous *N*,*N*′-dimethylformamide (5 mL) and anhydrous triethylamine (3 mL) as solvents, and stir at 45 °C for half an hour until the solution is clear, add 2-ethynylbenzoheterocycles **2a**-**2b** (1.000 mmol) and raise the temperature of the system to 70 °C. After the complete reaction, the solvent was concentrated under vacuum and reduced pressure to remove the solvent. Separation by column chromatography, (the eluent is dichloromethane: methanol = 10: 1) to afford compound **3a**-**3b**. The product **3a** was obtained as a dark brown solid in 60% yield.The product **3b** was obtained as a dark brown solid in 59% yield.

*1.2.4 Synthesis of Extended benzoheterocyclic 2-pyrrolidine (**4a-4b**)*

Add 5-(benzoheterocyclic ethynyl) cytidine (**3a**-**3b**) (0.500 mmol), ethanol (20 mL) into a 50 ml reaction flask and heat to 45 ºC; Then add sodium Chloroaurate dihydrate (0.068 mmol) solution dissolved in 2 mL ethanol into the system, raise the temperature to 70 °C and reflux for 24 hours; The reaction was tracked and monitored by TLC (the developing agent was acetonitrile: ammonia = 10: 1) to afford compound **4a**-**4b**. The product **4a** was obtained as a dark brown solid in 41% yield. The product **4b** was obtained as a dark brown solid in 42% yield.

***1.3 General procedure for formation of 4c-4d***



*1.3.1 Synthesis of 2-ethynyldibenzo[b,d]thiophene (**2c**)*

2-bromodibenzothiophene (150.0 mg, 0.570 mmol), bis(triphenylphosphine)palladium dichloride (44.0 mg, 0.063 mmol) and cuprous iodide (CuI) (12.0 mg, 0.063 mmol) were successively added to a 25 mL reaction flask. Vacuumize and fill with nitrogen for protection, add anhydrous triethylamine (4.0 mL) and toluene (4.0 mL) as solvent, stir at 80 ºC for half an hour, then add 2-methyl-3-butyne-2-alcohol (130.0 mg, 1.140 mmol), and continue the reaction for 15 hours. The solvent was removed by rotary distillation and separated by column chromatography (the eluent was hexane: ethyl acetate = 5: 1) to obtain the intermediate product 4-(dibenzo[b,d]thiophene-2-yl)-2-methyl-3-butyne-2-alcohol.4-(dibenzo[b,d]thiophene-2-yl)-2-methyl-3-butyne-2-ol (120.0 mg, 0.450 mmol), sodium hydride (34.6 mg, 1.440 mmol) and toluene (10.0 mL) were successively added into a 25 mL reaction flask and stirred for about 1 hour until the complete reaction (the reaction was tracked and monitored by TLC, and the developing agent was hexane: ethyl acetate = 5: 1). The solvent was removed by rotary evaporation and separated by column chromatography to afford compound **2c** (108 mg, 91%) as a dark brown solid.

*1.3.2 Synthesis of 2-ethynyldibenzo[b,d]furan (**2d**)*

Using 2-bromodibenzofuran as raw material, the experimental process is as follows: **2c**. The product **2d** was obtained as a dark brown solid (105 mg, 94%).

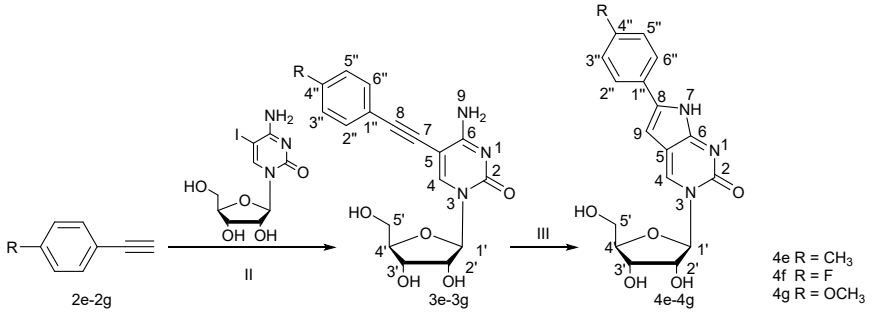
*1.3.3 Synthesis of 5-benzoheterocyclic ethynyl cytidine (**3c-3d**)*

Add 5-iodocarcidine (185 mg, 0.500 mmol), [1,1'-bis(diphenylphosphino)ferrocene] palladium dichloride (19.0 mg, 0.030 mmol) and cuprous iodide (CuI) (3.5 mg, 0.020 mmol) into a 25 mL reaction flask, anhydrous *N*,*N*'-dimethylformamide (5 mL) and anhydrous triethylamine (3 mL) as solvents, and stir at 45 °C for half an hour until the solution is clear, add 2-ethynylbenzoheterocycles **2c**-**2d** (1.000 mmol) and raise the temperature of the system to 70 °C. After the complete reaction, the solvent was concentrated under vacuum and reduced pressure to remove the solvent. Separation by column chromatography, (the eluent is dichloromethane: methanol = 10: 1) to afford compound **3c**-**3d**. The product **3c** was obtained as a dark brown solid in 55% yield.The product **3d** was obtained as a dark brown solid in 59% yield.

*1.3.4 Synthesis of Extended benzoheterocyclic 2-pyrrolidine (**4c-4d**)*

Add 5-(benzoheterocyclic ethynyl) cytidine (**3c**-**3d**) (0.500 mmol), ethanol (20 mL) into a 50 ml reaction flask and heat to 45 ºC; Then add sodium Chloroaurate dihydrate (0.068 mmol) solution dissolved in 2 mL ethanol into the system, raise the temperature to 70 °C and reflux for 24 hours; The reaction was tracked and monitored by TLC (the developing agent was acetonitrile: ammonia = 10: 1) to afford compound **4c**-**4d**. The product **4c** was obtained as a dark brown solid in 41% yield. The product **4d** was obtained as a dark brown solid in 40% yield.

***1.4 General procedure for formation of 4e-4g***



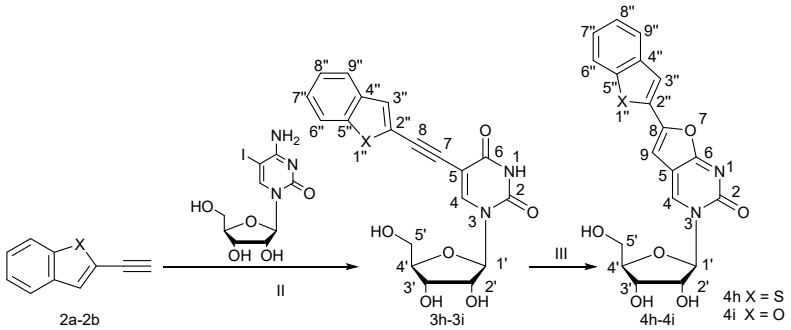
*1.4.1 Synthesis of 5-[(4-substituted phenyl)ethynyl)]cytidine (**3e-3g**)*

Under nitrogen, 5-iodocytidine (0.37 g, 1 mmol), [1,1'-bis(diphenylphosphino)ferrocene] palladium ($Pd(dppf)Cl_2$) (30 mg, 0.04 mmol) and copper iodide (CuI) (4.0 mg, 0.02 mmol) in a 50 mL reaction tube. Solvent anhydrous *N*,*N*-dimethylformamide (15 mL) and anhydrous triethylamine (3 mL) were added and the reaction was stirred at 45 °C for 1 hour. The solution turned a clear yellow solution. Then 4-substituted phenylethynyl (2 mmol) dissolved in 3 mL of triethylamine was added and the temperature was raised to 70 °C. The reaction was continued for 20 hours until the reaction was completed (TLC monitored the reaction). After the reaction was stopped, the reaction solution was concentrated under reduced pressure in vacuo, diluted with methanol (50 mL) and filtered off with suction to remove impurities. The filtrate was spin-dried and separated by column chromatography (column packed with 200-300 mesh silica gel, eluent dichloromethane: methanol = 10: 1) to give the product 5-(4-substituted phenylethynyl) cytidine (**3e**-**3g**). The product **3e** was a tan solid with a yield of 80%. The product **3f** is a brown solid in 85% yield.The product **3g** is a brown solid in 83% yield.

*1.4.2 Synthesis of 6-(4-substituted phenyl)-3-β-D-arabinofuranosyl-1,3-dihydro-2H pyrrolo[2,3-d]pyrimidin-2-one (**4e-4g**)*

5-[(4-Methylphenyl)ethynyl)]cytidine (**3e**-**3g**) (1 mmol) was added to a 100 mL single-necked flask and ethanol (20 mL) was added and heated to 45 °C. After adding a solution of NaAuCl4 $2H_2O$ (0.068 mmol) in ethanol (2 mL). The reaction temperature was raised to 70 °C and refluxed for 24 hours. The reaction was monitored by TLC (99/1, acetonitrile / ammonia). After the reaction was stopped, the solvent was removed by filtration and rotary evaporation. Through evaporation to dryness, the product (**4e**-g) was isolated and purified by column chromatography eluent: Vacetonitrile: Vammonia = 50: 1. The product **4e** was obtained as a light-yellow solid in 34% yield. The product **4f** was a yellow solid in 42% yield. The product **4g** was a yellow solid in 29% yield.

***1.5 General procedure for formation of 4h-4i***




*1.5.1 Synthesis of 5-benzoheterocyclic ethynyl uridine (**3h-3i**)*

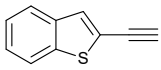
Add 5-iodonuridine (150.0 mg, 0.41 mmol), tetra (triphenylphosphine) palladium ($Pd[P(C_6H_5)_3]_4$) (47.3 mg, 0.04 mmol), cuprous iodide (CuI) (15.6 mg, 0.08 mmol) into a 25 mL reaction flask under nitrogen protection, anhydrous *N*,*N'*-dimethylformamide (5 mL) and anhydrous triethylamine (2.5 mL) as solvents, stir at room temperature for half an hour until the solution is clarified, add 2-ethynylbenzoheterocycles **2a**-**2b** (0.82 mmol) and continue the reaction. After the complete reaction, the solvent is concentrated under vacuum and reduced pressure, and separated by column chromatography (the leaching agent is dichloromethane: methanol = 10: 1) to afford compound **3h**-**3i**.

The product **3h** was obtained as a brown solid in 80% yield. The product **3i** was obtained as a light brown solid in 58% yield.

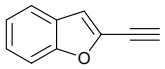
*1.5.2 Synthesis of extended benzoheterocyclic 2-furan uridine (**4h**-**4i**)*

Add 5-(benzoheterocyclic ethynyl) uridine (**3h**-**3i**) (150.0 mg, 0.37 mmol) and cuprous iodide (14.1 mg, 0.08 mmol) into a 50ml reaction flask, anhydrous methanol (15 mL) and anhydrous triethylamine (5 mL) as solvent, reflux at 65 ºC for 6 hours. After the reaction stops, the solvent is removed by spin evaporation; Separation and purification by column chromatography (leaching agent: dichloromethane: methanol = 10: 1), to yield compound (**4h**-**4i**). The product **4h** was obtained as a dark brown solid (64 mg, 41%). The product **4i** was obtained as a dark brown solid (62 mg, 41%).

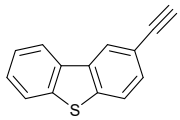
## 2. Characterization data for the compounds



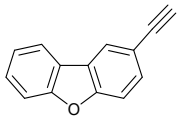
**2-ethynylbenzo[b]thiophene (2a):** $^{1}$H NMR (400 MHz, CDCl3): $\delta$ 7.83-7.77 (m, 2H), 7.55 (s, 1H), 7.41 (dd, $J$ = 7.3, 3.7 Hz, 2H), 3.48 (s, 1H). $^{13}$C NMR (101 MHz, CDCl3): $\delta$ 140.2, 138.8, 130.1, 125.8, 124.8, 124.0, 122.1, 83.0.



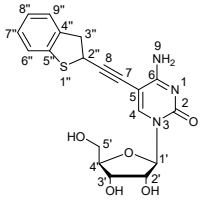
**2-ethynylbenzofuran (2b):** $^{1}$H NMR (400 MHz, DMSO): $\delta$ 7.66 (d, $J$ = 7.7 Hz, 1H), 7.58 (d, $J$ = 8.3 Hz, 1H), 7.40 (t, $J$ = 7.2 Hz, 1H), 7.30 (dd, $J$ = 13.3, 6.1 Hz, 2H), 4.94 (s, 1H). $^{13}$C NMR (101 MHz, DMSO): $\delta$ 154.6, 137.7, 127.4, 126.7, 124.1, 122.1, 113.1, 111.65, 88.1, 74.3.



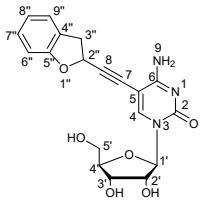
**Synthesis of 2-ethynyldibenzo[b,d]thiophene (2c):** $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.32 (d, $J$ = 1.1 Hz, 1H), 8.17-8.14 (m, 1H), 7.89-7.86 (m, 1H), 7.82 (d, $J$ = 8.6 Hz, 1H), 7.59 (dd, $J$ = 8.3, 1.5 Hz, 1H), 7.53-7.48 (m, 2H), 3.19 (s, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 140.1, 139.7, 135.6, 134.8, 130.1, 127.2, 125.4, 124.7, 122.8, 122.7, 121.7, 118.2, 83.9.



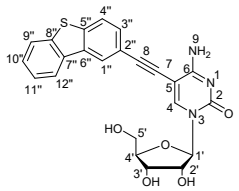
**Synthesis of 2-ethynyldibenzo[b,d]furan (2d):** $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.13 (d, $J$ = 1.3 Hz, 1H), 7.96 (d, $J$ = 8.2 Hz, 1H), 7.64-7.59 (m, 2H), 7.55-7.49 (m, 2H), 7.41-7.37 (m, 1H), 3.12 (s, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 156.6, 156.1, 133.7, 131.2, 128.7, 127.7, 124.7, 124.5, 123.5, 123.1, 120.8, 116.6, 111.8, 83.8.



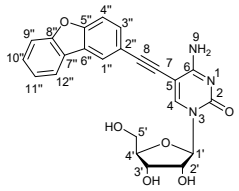
**4-amino-5-(benzo[b]thiophen-2-ylethynyl)-1-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl) -tetrahydrofuran-2-yl)pyrimidin-2(1H)-one (3a):** $^{1}$H NMR (400 MHz, DMSO): $\delta$ 8.51 (s, 1H), 7.99-7.94 (m, 1H), 7.89 (dd, $J$ = 6.2, 2.9 Hz, 2H), 7.78 (s, 1H), 7.46-7.40 (m, 2H), 7.24 (s, 1H), 5.80 (d, $J$ = 2.8 Hz, 1H), 5.42 (s, 1H), 5.26 (s, 1H), 5.03 (s, 1H), 4.00 (s, 2H), 3.88 (d, $J$ = 2.5 Hz, 1H), 3.76 (d, $J$ = 12.0 Hz, 1H), 3.60 (d, $J$ = 8.7 Hz, 1H). $^{13}$C NMR (101 MHz, DMSO): $\delta$ 164.0, 154.0, 146.5, 139.9, 139.2, 130.0, 126.2, 125.5, 124.5, 122.8, 122.7, 90.0, 89.5, 87.8, 87.7, 84.6, 74.8, 69.3, 60.5.



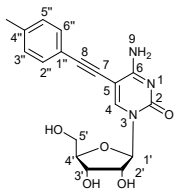
**4-amino-5-(benzofuran-2-ylethynyl)-1-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetra-hydrofuran-2-yl)pyrimidin-2(1H)-one (3b):** $^{1}$H NMR (400 MHz, DMSO): $\delta$ 8.58 (s, 1H), 7.88 (s, 1H), 7.70 (d, $J$ = 7.5 Hz, 1H), 7.60 (d, $J$ = 8.3 Hz, 1H), 7.40 (t, $J$ = 7.7 Hz, 1H), 7.35 (d, $J$ = 0.7 Hz, 1H), 7.31 (t, $J$ = 7.5 Hz, 1H),7.20(s, 1H), 5.80 (d, $J$ = 2.6 Hz, 1H), 5.43 (d, $J$ = 4.5 Hz, 1H), 5.26 (t, $J$ = 4.8 Hz, 1H), 5.01 (d, $J$ = 5.2 Hz, 1H), 4.00 (s, 2H), 3.92-3.85 (m, 1H), 3.79-3.71 (m, 1H), 3.64-3.56 (m, 1H). $^{13}$C NMR (101 MHz, DMSO): $\delta$ 164.0, 154.7, 153.9, 147.1, 138.6, 127.8, 126.4, 124.1, 122.0, 112.8, 111.5, 90.2, 88.6, 88.2, 84.6, 84.5, 74.9, 69.2, 60.4.



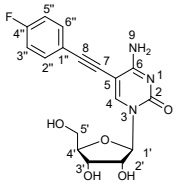
**4-amino-5-(dibenzo[b,d]thiophen-2-ylethynyl)-1-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxy-methyl) tetrahydrofuran-2-yl)pyrimidin-2(1H)-one (3c):** $^{1}$H NMR (400 MHz, DMSO): $\delta$ 8.63 (d, $J$ = 1.0 Hz, 1H), 8.54 (s, 1H), 8.38 (dd, $J$ = 6.3, 2.8 Hz, 1H), 8.13-8.02 (m, 2H), 7.90 (s, 1H), 7.72 (dd, $J$ = 8.3, 1.5 Hz, 1H), 7.63-7.49 (m, 2H), 7.16 (s, 1H), 5.83 (s, 1H), 5.45 (s, 1H), 5.34 (s, 1H), 5.08 (s, 1H), 4.04 (dd, $J$ = 8.4, 4.4 Hz, 2H), 3.96-3.86 (m, 1H), 3.83-3.73 (m, 1H), 3.69-3.58 (m, 1H). $^{13}$C NMR (101 MHz, DMSO): $\delta$ 164.3, 154.1, 145.8, 139.4, 139.2, 135.6, 134.9, 130.1, 128.0, 125.5, 125.3, 123.7, 122.6, 119.4, 94.4, 90.1, 90.0, 84.6, 82.1, 74.9, 69.3, 60.5.



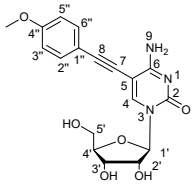
**4-amino-5-(dibenzo[b,d]furan-2-ylethynyl)-1-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)-tetrahydrofuran -2-yl)pyrimidin-2(1H)-one (3d):** $^{1}$H NMR (400 MHz, DMSO): $\delta$ 8.51 (s, 1H), 8.43 (s, 1H), 8.15 (d, $J$ = 7.4 Hz, 1H), 7.86-7.71 (m, 3H), 7.60-7.53 (m, 1H), 7.45 (t, $J$ = 7.5 Hz, 1H), 7.16 (s, 1H), 5.83 (d, $J$ = 3.1 Hz, 1H), 5.76 (s, 1H), 5.44 (d, $J$ = 4.3 Hz, 1H), 5.32 (t, $J$ = 4.7 Hz, 1H), 5.07 (d, $J$ = 4.8 Hz, 1H), 4.03 (d, $J$ = 3.1 Hz, 2H), 3.93-3.87 (m, 1H), 3.81-3.73 (m, 1H), 3.67-3.59 (m, 1H). $^{13}$C NMR (101 MHz, DMSO): $\delta$ 164.3, 156.4, 155.5, 154.2, 145.7, 131.4, 128.6, 124.8, 124.3, 124.0, 123.4, 121.8, 117.9, 112.5, 112.3, 94.2, 90.0, 84.6, 81.2, 74.9, 69.4, 60.5, 55.4.



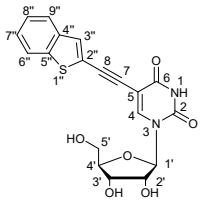
**4-amino-1-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-(p-tolyl-ethynyl)pyrimidin-2(1H)-one (3e):** $^{1}$H NMR (400 MHz, DMSO-d6) $\delta$ 8.44 (s, 1H), 7.80 (s, 1H),7.48 (d, $J$ = 8.0 Hz, 2H), 7.21 (d, $J$ = 8.0 Hz, 2H), 7.05 (s, 1H), 5.79 (s, 1H), 5.41 (s, 1H), 5.25 (s, 1H), 5.03 (s, 1H), 3.98 (s, 2H), 3.87 (s, 1H), 3.69 (s, 1H), 3.59 (s, 1H), 2.33 (s, 3H). 13C NMR (101 MHz, DMSO): $\delta$ 164.3, 154.1, 145.6, 138.6, 131.6, 129.6, 119.8, 94.3, 90.0, 84.6, 81.4, 74.8, 69.3, 60.5, 21.3.



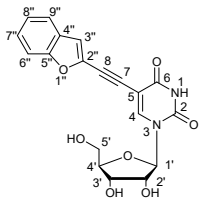
**4-amino-1-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-((4-fluoro-phenyl)ethynyl)pyrimidin-2(1H)-one (3f):** $^{1}$H NMR (400 MHz, DMSO-d6) $\delta$ 8.47 (s, 1H), 7.81 (s, 1H), 7.64 (s, 2H), 7.27 (t, $J$ = 8.9 Hz, 2H), 7.11 (s, 1H), 5.78 (d, $J$ = 3.0 Hz, 1H), 5.40 (d, $J$ = 4.6 Hz, 1H), 5.25 (t, $J$ = 4.7 Hz, 1H), 5.01 (d, $J$ = 5.2 Hz, 1H), 3.99 (s, 2H), 3.86 (s, 1H), 3.74 (s, 1H), 3.61 (s, 1H). $^{13}$C NMR (101 MHz, DMSO-d6) $\delta$ 164.2, 163.6, 154.1, 145.9, 134.0, 140.0,119.4, 116.3, 116.1, 93.1, 90.0, 84.5, 81.8, 74.8, 69.3, 60.4.



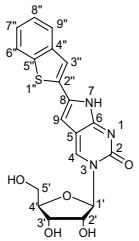
**4-amino-1-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-5-((4-methoxyphenyl)ethynyl)pyrimidin-2(1H)-one (3g):** $^{1}$H NMR (400 MHz, DMSO-d6) $\delta$ 8.39 (s, 1H), 7.77 (s, 1H), 7.53 (d, $J$ = 11.5 Hz, 2H), 7.01 (s, 1H), 6.98 (s, 1H), 6.95 (s, 1H), 5.79 (s, 1H), 5.39 (s, 1H), 5.23 (s, 1H), 5.00 (s, 1H), 3.98 (s, 2H), 3.89-3.84 (m, 1H), 3.79 (s, 3H), 3.71 (s, 1H), 3.61 (s, 1H). $^{13}$C NMR (101 MHz, DMSO-d6) $\delta$ 161.9, 160.1, 150.2, 144.0, 133.2, 114.8, 114.8, 99.1, 92.4, 88.8, 85.2, 81.2, 74.4, 69.7, 60.7, 55.7.



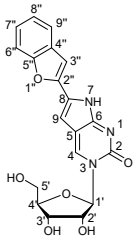
**5-(benzo[b]thiophen-2-ylethynyl)-1-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydro-furan-2-yl)pyrimidine-2,4(1H,3H)-dione (3h):** $^{1}$H NMR (400 MHz, DMSO): $\delta$ 11.80 (s, 1H), 8.55 (s, 1H), 7.99-7.93 (m, 1H), 7.90-7.84 (m, 1H), 7.69 (s, 1H), 7.46-7.41 (m, 2H), 5.79 (d, $J$ = 4.4 Hz, 1H), 5.48 (d, $J$ = 5.3 Hz, 1H), 5.30 (t, $J$ = 4.8 Hz, 1H), 5.10 (d, $J$ = 5.5 Hz, 1H), 4.10 (dd, $J$ = 9.6, 4.8 Hz, 1H), 4.04 (dd, $J$ = 10.0, 5.0 Hz, 1H), 3.93-3.87 (m, 1H), 3.72 (dd, $J$ = 9.9, 6.5 Hz, 1H), 3.65-3.58 (m, 1H). $^{13}$C NMR (101 MHz, DMSO): $\delta$ 161.7, 150.1, 145.2, 139.3, 139.3, 129.6, 126.4, 125.6, 124.6, 122.8, 122.5, 98.1, 89.1, 88.6, 85.7, 85.2, 74.4, 69.7, 60.7.



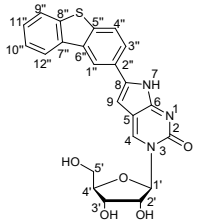
**5-(benzofuran-2-ylethynyl)-1-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)pyrimidine-2,4(1H,3H)-dione (3i):** $^{1}$H NMR (400 MHz, DMSO): $\delta$ 11.83 (s, 1H), 8.61 (s, 1H), 7.67 (d, $J$ = 7.7 Hz, 1H), 7.58 (d, $J$ = 8.3 Hz, 1H), 7.43-7.37 (m, 1H), 7.35-7.27 (m, 2H), 5.78 (d, $J$ = 4.3 Hz, 1H), 5.48 (d, $J$ = 5.2 Hz, 1H), 5.31 (t, $J$ = 4.8 Hz, 1H), 5.11 (d, $J$ = 5.5 Hz, 1H), 4.10 (dd, $J$ = 9.6, 4.8 Hz, 1H), 4.04 (dd, $J$ = 10.3, 5.1 Hz, 1H), 3.93-3.88 (m, 1H), 3.75 (ddd, $J$ = 11.8, 4.4, 3.0 Hz, 1H), 3.63 (ddd, $J$ = 12.0, 4.4, 2.8 Hz, 1H).$^{13}$C NMR (101 MHz, DMSO): $\delta$ 161.6, 154.7, 150.0, 145.8, 138.2, 127.7, 126.5, 124.1, 122.1, 112.4, 111.6, 97.3, 89.2, 89.1, 85.2, 82.5, 74.5, 69.6, 60.5.



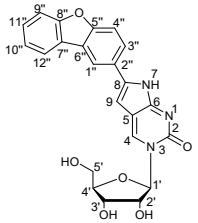
**6-(benzo[b]thiophen-2-yl)-3-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-3,7-dihydro-2H-pyrrolo[2,3-d]pyrimidin-2-one (4a):** $^{1}$H NMR (400 MHz, DMSO): $\delta$ 12.10 (s, 1H), 8.88 (s, 1H), 7.98-7.95 (m, 1H), 7.96 (s, 1H), 7.85-7.82 (m, 1H), 7.39 (dd, $J$ = 7.4, 2.0 Hz, 2H), 6.60 (s, 1H), 5.95 (s, 1H), 5.54 (s, 1H), 5.32 (s, 1H), 5.10 (d, $J$ = 4.0 Hz, 1H), 4.06-3.99 (m, 3H), 3.82 (d, $J$ = 10.8 Hz, 1H), 3.70 (d, $J$ = 11.9 Hz, 1H). $^{13}$C NMR (101 MHz, DMSO): $\delta$ 160.3, 154.6, 154.0, 140.2, 138.9, 138.0, 134.1, 130.0, 125.5, 124.4, 122.9, 121.6, 109.4, 99.5, 91.7, 84.7, 75.5, 69.0, 60.4.



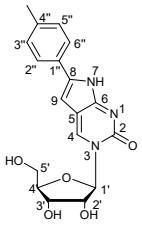
**6-(benzofuran-2-yl)-3-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-3,7-dihydro-2H-pyrrolo[2,3-d]pyrimidin-2-one (4b):** $^{1}$H NMR (400 MHz, DMSO): $\delta$ 12.11 (s, 1H), 8.93 (s, 1H), 7.69 (d, $J$ = 7.5 Hz, 1H), 7.60 (d, $J$ = 8.2 Hz, 1H), 7.39-7.32 (m, 2H), 7.28 (t, $J$ = 7.4 Hz, 1H), 6.71 (s, 1H), 5.96 (s, 1H), 5.57 (s, 1H), 5.31 (s, 1H), 5.08 (s, 1H), 4.05 (d, $J$ = 22.0 Hz, 3H), 3.86 (d, $J$ = 11.9 Hz, 1H), 3.70 (d, $J$ = 12.0 Hz, 1H). $^{13}$C NMR (101 MHz, DMSO): $\delta$ 160.2, 154.8, 154.6, 148.4, 138.5, 130.6, 128.7, 125.7, 124.0, 122.0, 111.5, 109.2, 104.1, 99.0, 91.8, 84.7, 75.5, 69.0, 60.4.



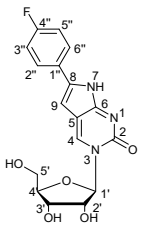
**6-(dibenzo[b,d]thiophen-2-yl)-3-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-3,7-dihydro-2H-pyrrolo[2,3-d]pyrimidin-2-one (4c):** $^{1}$H NMR (400 MHz, DMSO): $\delta$ 11.89 (s, 1H), 8.63 (s, 1H), 8.53 (s, 1H), 8.37 (d, $J$ = 6.3, 2.8 Hz, 1H), 8.09-8.07 (t, $J$ = 7.8 Hz, 2H), 7.71 (d, $J$ = 8.3, 1.5 Hz, 1H), 7.57-7.13 (d, $J$ = 5.9, 3.3 Hz, 2H), 6.94 (d, $J$ = 76.8 Hz, 1H), 5.82 (d, $J$ = 3.2 Hz, 1H), 5.43 (d, $J$ = 52.9 Hz, 2H), 5.05 (s, 1H), 4.02 (s, 2H), 3.93-3.87 (m, 1H), 3.77 (d, $J$ = 11.9 Hz, 1H), 3.65 (d, $J$ = 12.0 Hz, 1H). $^{13}$C NMR (101 MHz, DMSO): $\delta$ 164.3, 154.1, 145.8, 139.4, 139.2, 135.6, 134.9, 130.1, 128.0, 125.5, 125.2, 123.7, 122.6, 119.4, 94.4, 90.1, 90.0, 84.5, 82.1, 74.9, 69.3, 60.4, 56.5.



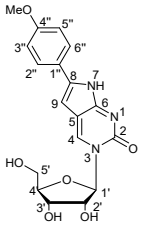
**6-(dibenzo[b,d]furan-2-yl)-3-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)-3,7-dihydro-2H-pyrrolo[2,3-d]pyrimidin-2-one (4d):** $^{1}$H NMR (400 MHz, DMSO): $\delta$ 11.87 (s, 1H), 8.89 (s, 1H), 8.68 (s, 1H), 8.12 (d, $J$ = 7.6 Hz, 1H), 8.03 (d, $J$ = 8.6 Hz, 1H), 7.79 (dd, $J$ = 16.9, 8.4 Hz, 2H), 7.57-7.46 (dt, $J$ = 42.1, 7.5 Hz, 2H), 6.81 (s, 1H), 5.98 (d, $J$ = 2.0 Hz, 1H), 5.66-5.06 (m, 3H), 4.06 (s, 2H), 4.02-3.96 (m, 1H), 3.84 (d, $J$ = 12.1 Hz, 1H), 3.71 (d, $J$ = 13.6 Hz, 1H). $^{13}$C NMR (101 MHz, DMSO): $\delta$ 160.6, 156.4, 155.7, 154.6, 140.1, 137.1, 128.5, 126.5, 125.5, 124.6, 123.9, 123.8, 121.6, 118.3, 112.6, 112.4, 109.8, 97.0, 91.7, 84.5, 75.5, 68.8, 60.2.



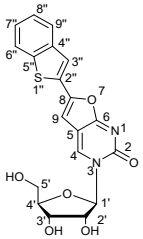
**3-*β*-D-arabinofuranosyl-6-(4-methylphenyl)-1,3-dihydro-2H-pyrrolo[2,3-d] pyrimidin-2-one (4e):** $^{1}$H NMR (400 MHz, DMSO-d6) $\delta$ 11.75 (s, 1H), 8.81 (s, 1H), 7.73 (d, $J$ = 8.1 Hz, 2H), 7.26 (d, $J$ = 8.1 Hz, 2H), 6.66 (s, 1H), 5.95 (s, 1H), 5.50 (s, 1H), 5.34 (s, 1H), 5.10 (s, 1H), 4.03 (s, 2H), 3.98-3.94 (m, 1H), 3.79 (s, 1H), 3.65 (s, 1H), 2.33 (s, 3H). $^{13}$C NMR (101 MHz, DMSO-d6) $\delta$ 160.5, 154.6, 140.1, 138.4, 136.9, 129.9, 128.3, 125.5, 96.6, 91.6, 84.6, 75.5, 69.0, 60.3, 21.3.



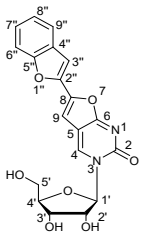
**3-*β*-D-arabinofuranosyl-6-(4-fluorophenyl)-1,3-dihydro-2H-pyrrolo[2,3-d] pyrimidin-2-one (4f):** $^{1}$H NMR (400 MHz, DMSO-d6) $\delta$ 11.82 (s, 1H), 8.85 (s, 1H), 8.01-7.82 (m, 2H), 7.32-7.27 (m, 2H), 6.71 (s, 1H), 5.95 (s, 1H), 5.50 (s, 1H), 5.33 (s, 1H), 5.08 (s, 1H), 4.03-3.97 (d, $J$ = 25.6 Hz, 3H), 3.82 (d, $J$ = 10.6 Hz, 1H), 3.71-3.56 (m, 1H). $^{13}$C NMR (101 MHz, DMSO-d6) $\delta$ 160.4, 154.8, 149.3, 139.0, 137.4, 134.0, 127.8, 116.4, 116.2, 109.7, 97.6, 91.5, 84.6, 75.5, 68.945, 60.0.



**3-*β*-D-arabinofuranosyl-6-(4-methoxylphenyl)-1,3-dihydro-2H-pyrrolo[2,3-d] pyrimidin-2-one (4g):** $^{1}$H NMR (400 MHz, DMSO-d6) $\delta$ 11.71 (s, 1H), 8.76 (s, 1H), 7.80 (d, $J$ = 8.6 Hz, 2H), 7.02 (d, $J$ = 8.6 Hz, 2H), 6.58 (s, 1H), 5.96 (s, 1H), 5.50 (s, 1H), 5.29 (s, 1H), 5.05 (s, 1H), 4.03 (s, 2H), 3.96 (s, 1H), 3.80 (s, 3H), 3.72-3.61 (m, 1H). $^{13}$C NMR (101 MHz, DMSO-d6): $\delta$ 163.6, 159.9, 153.2, 145.6, 133.4, 114.8, 114.6, 94.4, 90.6, 89.9, 84.6, 80.0, 74.8, 69.3, 60.4, 55.6.



**6-(benzo[b]thiophen-2-yl)-3-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl)furo[2,3-d]pyrimidin-2(3H)-one (4h):** $^{1}$H NMR (400 MHz, DMSO): $\delta$ 9.05 (s, 1H), 8.05-8.01 (m, 1H), 7.95 -7.90 (m, 2H), 7.44-7.40 (m, 2H), 7.24 (s, 1H), 5.88 (s, 1H), 5.64 (s, 1H), 5.41 (s, 1H), 5.14 (s, 1H), 4.07-4.00 (m, 3H), 3.85 (d, $J$ = 12.2 Hz, 1H), 3.71 (d, $J$ = 12.0 Hz, 1H). $^{13}$C NMR (101 MHz, DMSO): $\delta$ 171.4, 154.4, 149.2, 139.9, 139.6, 139.3, 130.8, 126.2, 125.7, 124.9, 123.1, 122.8, 107.1, 101.7, 92.2, 84.7, 75.4, 68.5, 59.9.



**6-(benzofuran-2-yl)-3-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)tetrahydrofuran-2-yl) furo[2,3-d]pyrimidin-2(3H)-one (4i):** $^{1}$H NMR (400 MHz, DMSO): $\delta$ 8.62 (s, 1H), 7.68 (d, $J$ = 7.5 Hz, 1H), 7.60 (d, $J$ = 8.2 Hz, 1H), 7.41 (dd, $J$ = 13.8, 6.5 Hz, 2H), 7.33-7.22 (m, 2H), 5.50 (s, 1H), 5.33 (s, 1H), 5.31 (s, 1H), 5.13 (d, $J$ = 19.6 Hz, 1H), 5.11 (s, 1H), 5.07(m,2H), 4.03 (s, 1H), 3.95 (s, 1H). $^{13}$C NMR (101 MHz, DMSO): $\delta$ 161.6, 154.7, 150.0, 145.8, 140.1, 138.3, 127.7, 126.5, 124.1, 122.1, 112.4, 111.6, 97.3, 89.3, 89.1, 85.2, 74.5, 69.6, 60.6.

## 3. Spectra data of absorption and emission

Tab.1 Uv.-vis. spectra data of **4a**~**4i** in pH solutions

| pH | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $\lambda_{max}$(nm) | **4a** | 385 | 372 | 373 | 376 | 376 | 374 | 377 | 376 | 377 | 376 | 377 | 382 |
| | **4b** | 390 | 376 | 374 | 374 | 374 | 374 | 374 | 373 | 374 | 373 | 374 | 381 |
| | **4c** | 389 | 389 | 389 | 387 | 389 | 389 | 389 | 389 | 389 | 390 | 390 | 389 |
| | **4d** | 386 | 380 | 364 | 369 | 369 | 373 | 374 | 373 | 371 | 366 | 372 | 372 |
| | **4e** | 373 | 363 | 363 | 363 | 363 | 363 | 362 | 362 | 361 | 363 | 364 | 370 |
| | **4f** | 368 | 361 | 361 | 360 | 360 | 361 | 361 | 361 | 360 | 360 | 360 | 368 |
| | **4g** | 383 | 372 | 367 | 366 | 366 | 366 | 366 | 366 | 366 | 366 | 368 | 376 |
| | **4h** | 356 | 357 | 355 | 357 | 355 | 355 | 356 | 351 | 349 | 349 | 349 | - |
| | **4i** | 356 | 356 | 355 | 357 | 356 | 355 | 356 | 351 | 350 | 349 | 349 | - |
| $\varepsilon$ ($10^3M^{-1}cm^{-1}$) | **4a** | 6.0 | 7.2 | 6.0 | 5.4 | 5.3 | 5.4 | 5.3 | 5.4 | 5.7 | 5.9 | 6.5 | 5.0 |
| | **4b** | 6.6 | 8.0 | 8.9 | 9.1 | 8.8 | 9.0 | 9.0 | 9.0 | 8.8 | 7.8 | 7.8 | 6.2 |
| | **4c** | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.6 | 0.5 | 0.5 | 0.7 |
| | **4d** | 1.2 | 1.2 | 1.2 | 1.2 | 1.2 | 1.2 | 1.2 | 1.2 | 1.2 | 1.2 | 1.1 | 1.1 |
| | **4e** | 1.19 | 1.38 | 1.41 | 1.41 | 1.46 | 1.42 | 1.39 | 1.37 | 1.32 | 1.23 | 1.18 | 0.85 |
| | **4f** | 3.44 | 3.55 | 3.70 | 3.55 | 3.45 | 3.53 | 3.68 | 3.76 | 3.74 | 3.54 | 3.09 | 2.17 |
| | **4g** | 2.58 | 3.03 | 3.42 | 3.33 | 3.42 | 3.40 | 3.57 | 3.50 | 3.43 | 3.10 | 2.70 | 2.19 |
| | **4h** | 3.2 | 2.7 | 2.9 | 2.9 | 2.9 | 2.9 | 2.9 | 2.9 | 2.6 | 2.3 | 2.5 | - |
| | **4i** | 3.1 | 2.7 | 2.7 | 2.7 | 2.7 | 2.7 | 2.8 | 2.8 | 2.5 | 2.4 | 2.4 | - |

Tab.2 Fluorescence spectra data of **4a**~**4i** in pH solutions

| pH | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $\lambda_{em}$(nm) | **4a** | 516 | 464 | 464 | 463 | 466 | 467 | 465 | 463 | 465 | 465 | 465 | 453 |
| | **4b** | 531 | 467 | 469 | 469 | 471 | 469 | 469 | 469 | 469 | 469 | 467 | 467 |
| | **4c** | 526 | 477 | 467 | 471 | 467 | 467 | 467 | 471 | 465 | 471 | 471 | 475 |
| | **4d** | 523 | 475 | 473 | 469 | 469 | 469 | 467 | 467 | 469 | 469 | 469 | 465 |
| | **4e** | 520 | 469 | 470 | 468 | 467 | 469 | 465 | 466 | 466 | 467 | 468 | 472 |
| | **4f** | 501 | 465 | 465 | 464 | 465 | 464 | 467 | 463 | 464 | 464 | 464 | 462 |
| | **4g** | 540 | 478 | 475 | 477 | 479 | 480 | 477 | 482 | 476 | 481 | 478 | 480 |
| | **4h** | 463 | 461 | 461 | 467 | 465 | 461 | 467 | 467 | 471 | 463 | 467 | 467 |
| | **4i** | 467 | 471 | 469 | 467 | 473 | 469 | 473 | 469 | 469 | 469 | 471 | 469 |
| *Intensity* (a.u.) | **4a** | 8.2 | 70.4 | 235.1 | 272.6 | 237.6 | 255.0 | 277.8 | 296 | 291.5 | 275.5 | 200.5 | 56.6 |
| | **4b** | 8.4 | 96 | 347.9 | 419.6 | 341.2 | 380.0 | 452 | 469 | 487.4 | 462.5 | 286.1 | 71.8 |
| | **4c** | 10.7 | 56 | 178.5 | 222.4 | 227.7 | 214.0 | 237.7 | 238.2 | 242.7 | 204.1 | 195.3 | 120.6 |
| | **4d** | 49.6 | 278.8 | 724 | 775.5 | 143.5 | 794.0 | 822.5 | 853.4 | 743.5 | 942.3 | 743.5 | 495.7 |
| | **4e** | 1.85 | 19.35 | 61.66 | 78.89 | 77.99 | 82.9 | 85.5 | 86.85 | 91.91 | 88.37 | 69.19 | 15.41 |
| | **4f** | 22.83 | 182.5 | 695.6 | 861.9 | 901 | 926.5 | 980.9 | 956.9 | 978.9 | 932.6 | 647.1 | 170.7 |
| | **4g** | 12.83 | 178.2 | 576.7 | 755.3 | 731.4 | 819.0 | 845.5 | 840.8 | 842.1 | 870.7 | 696.1 | 156.5 |
| | **4h** | 18.2 | 122.2 | 206.5 | 220.7 | 204.5 | 206.5 | 218.6 | 213.9 | 225 | 220.9 | 215.4 | 208.9 |
| | **4i** | 38.4 | 199.7 | 398.8 | 435.7 | 416.8 | 419.0 | 439.1 | 460.2 | 454.6 | 445.9 | 426.3 | 341.9 |

Tab. 3 UV-vis. spectra data of **4a**~**4i** in different viscosity solutions

| viscosity（Pa·s） | | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** |
|---|---|---|---|---|---|---|---|---|---|---|
| | | 0.58 | 4.43 | 6.36 | 13.38 | 30.27 | 55.13 | 190.62 | 329.84 | 468.14 |
| $\lambda_{max}$ (nm) | **4a** | 376 | 378 | 378 | 378 | 378 | 378 | 378 | 379 | 379 |
| | **4b** | 376 | 376 | 377 | 377 | 377 | 377 | 378 | 378 | 378 |
| | **4c** | 369 | 368 | 372 | 371 | 370 | 370 | 371 | 373 | 372 |
| | **4d** | 368 | 367 | 368 | 369 | 369 | 369 | 369 | 369 | 369 |
| | **4e** | 365 | 366 | 364 | 366 | 367 | 366 | 367 | 367 | 367 |
| | **4f** | 363 | 364 | 364 | 364 | 363 | 363 | 364 | 365 | 366 |
| | **4g** | 370 | 370 | 371 | 369 | 371 | 371 | 372 | 372 | 373 |
| | **4h** | 363 | 363 | 363 | 363 | 363 | 363 | 364 | 366 | 366 |
| | **4i** | 362 | 363 | 363 | 363 | 363 | 364 | 364 | 364 | 363 |
| $\varepsilon$ ($10^3 M^{-1}cm^{-1}$) | **4a** | 6.7 | 6.7 | 6.8 | 6.6 | 6.6 | 6.7 | 6.4 | 6.6 | 7.5 |
| | **4b** | 7.3 | 7.0 | 7.1 | 7.0 | 7.3 | 7.2 | 6.7 | 7.9 | 7.2 |
| | **4c** | 1.7 | 1.9 | 2.1 | 1.9 | 1.8 | 1.7 | 2.0 | 1.8 | 2.0 |
| | **4d** | 5.0 | 5.3 | 5.7 | 5.3 | 5.3 | 5.3 | 5.7 | 5.6 | 5.6 |
| | **4e** | 3.3 | 3.4 | 3.3 | 3.4 | 3.3 | 3.4 | 3.5 | 3.7 | 3.7 |
| | **4f** | 4.7 | 4.2 | 4.2 | 4.5 | 4.3 | 4.1 | 4.8 | 4.6 | 4.9 |
| | **4g** | 6.1 | 6.3 | 6.0 | 6.7 | 6.8 | 6.5 | 6.4 | 6.3 | 6.7 |
| | **4h** | 8.4 | 8.8 | 9.0 | 9.0 | 9.1 | 8.6 | 8.7 | 9.1 | 8.8 |
| | **4i** | 8.8 | 9.2 | 9.3 | 9.3 | 9.4 | 9.0 | 9.1 | 9.5 | 9.4 |

Tab. 4 Emission peaks and fluorescence intensity in different viscosity solutions

| viscosity（Pa·s） | | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** |
|---|---|---|---|---|---|---|---|---|---|---|
| | | 0.58 | 4.43 | 6.36 | 13.38 | 30.27 | 55.13 | 190.62 | 329.84 | 468.14 |
| $\lambda_{em}$ (nm) | **4a** | 455 | 455 | 457 | 455 | 457 | 457 | 457 | 455 | 455 |
| | **4b** | 455 | 459 | 459 | 459 | 459 | 459 | 461 | 461 | 459 |
| | **4c** | 459 | 463 | 459 | 463 | 463 | 463 | 463 | 463 | 463 |
| | **4d** | 459 | 459 | 459 | 461 | 461 | 461 | 461 | 461 | 461 |
| | **4e** | 455 | 456 | 459 | 461 | 461 | 458 | 459 | 461 | 463 |
| | **4f** | 451 | 453 | 454 | 452 | 455 | 455 | 457 | 459 | 459 |
| | **4g** | 460 | 468 | 462 | 465 | 468 | 467 | 468 | 469 | 471 |
| | **4h** | 442 | 448 | 448 | 450 | 444 | 446 | 450 | 449 | 444 |
| | **4i** | 445 | 447 | 446 | 449 | 453 | 447 | 445 | 451 | 447 |
| Intensity (a.u.) | **4a** | 486.1 | 499.6 | 496.3 | 501.8 | 516.8 | 510.7 | 500.6 | 480.8 | 441.5 |
| | **4b** | 919.1 | 951.1 | 967.0 | 959.9 | 945.3 | 911.4 | 908.5 | 908.5 | 910.7 |
| | **4c** | 693.8 | 708.8 | 699.0 | 711.1 | 685.2 | 672.8 | 647.4 | 638.9 | 645.4 |
| | **4d** | 387.7 | 401.9 | 410.6 | 405.3 | 386.7 | 378.5 | 383.7 | 377.5 | 381.3 |
| | **4e** | 536.6 | 590.5 | 603.9 | 622.9 | 634.6 | 632.0 | 621.8 | 585.5 | 558.9 |
| | **4f** | 164.7 | 181.5 | 186.3 | 194.5 | 197.4 | 199.4 | 195.6 | 187.9 | 182.9 |
| | **4g** | 559.5 | 618.3 | 629.5 | 656.0 | 633.9 | 598.1 | 610.5 | 567.6 | 549.6 |
| | **4h** | 389.5 | 347.4 | 224.2 | 369.1 | 333.5 | 327.4 | 297.2 | 306.7 | 323.4 |
| | **4i** | 628.1 | 731.3 | 698.7 | 721.1 | 729.2 | 731.0 | 728.7 | 689.5 | 625.3 |

## 4. Fluorescence lifetime

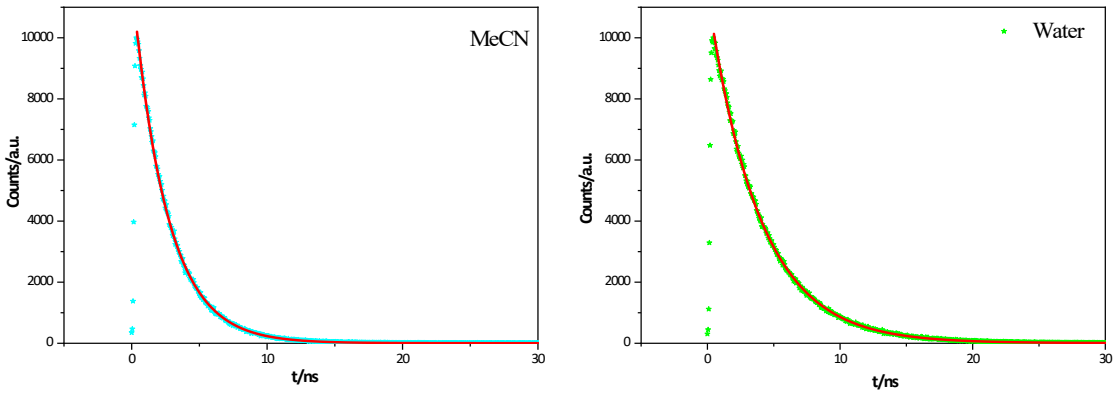



Figure 1. Fluorescence lifetime decay curves of **4a** in polarity solvents

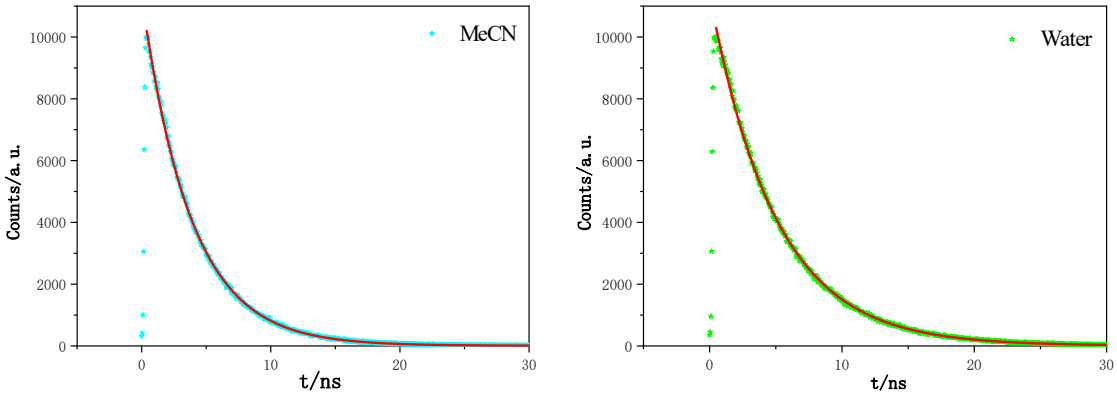



Figure 2. Fluorescence lifetime decay curves of **4b** in polarity solvents

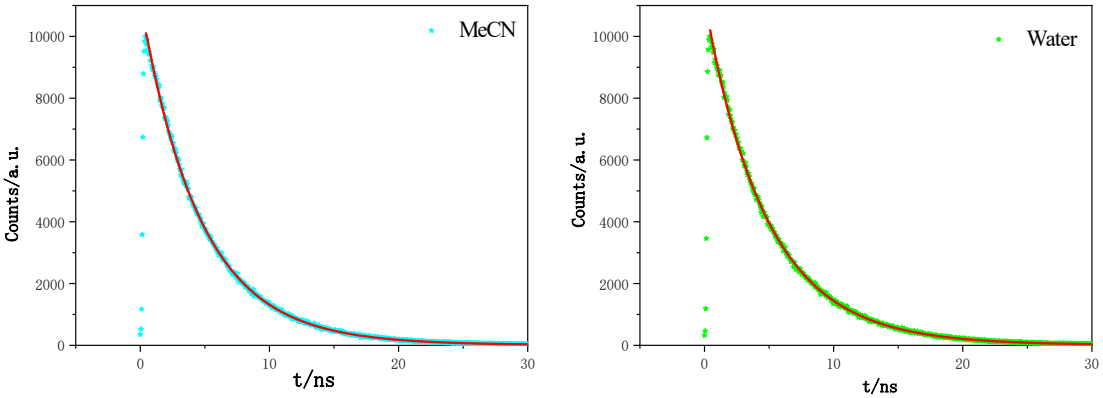



Figure 3. Fluorescence lifetime decay curves of **4c** in polarity solvents

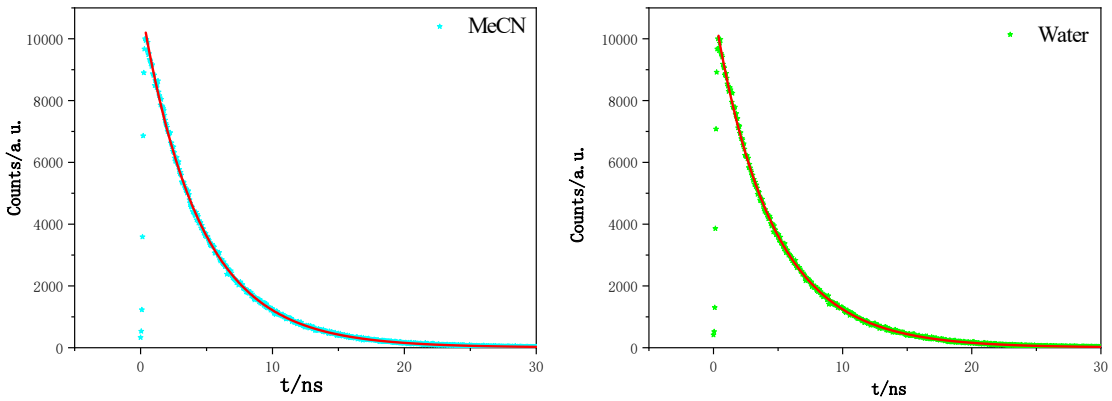



Figure 4. Fluorescence lifetime decay curves of **4d** in polarity solvents

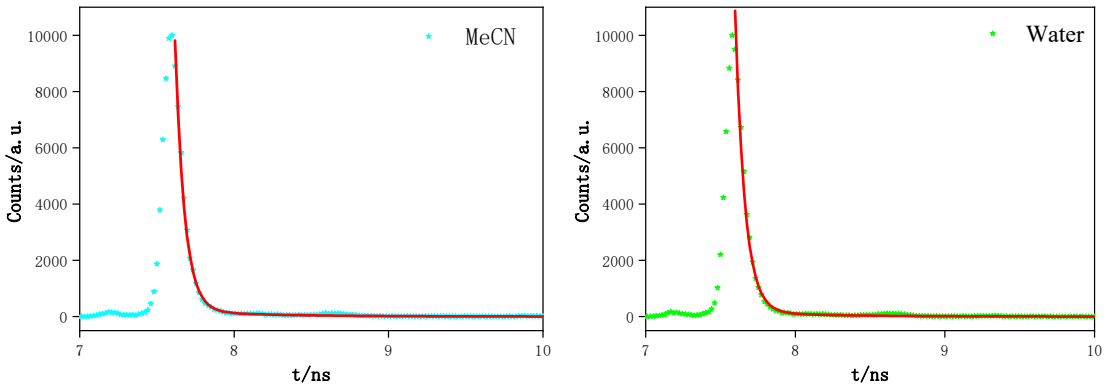



Figure 5. Fluorescence lifetime decay curves of **4e** in polarity solvents

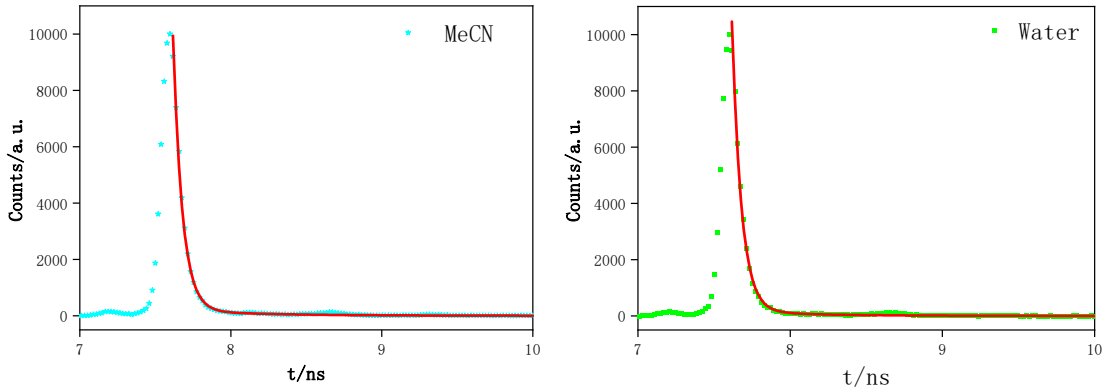



Figure 6. Fluorescence lifetime decay curves of **4f** in polarity solvents

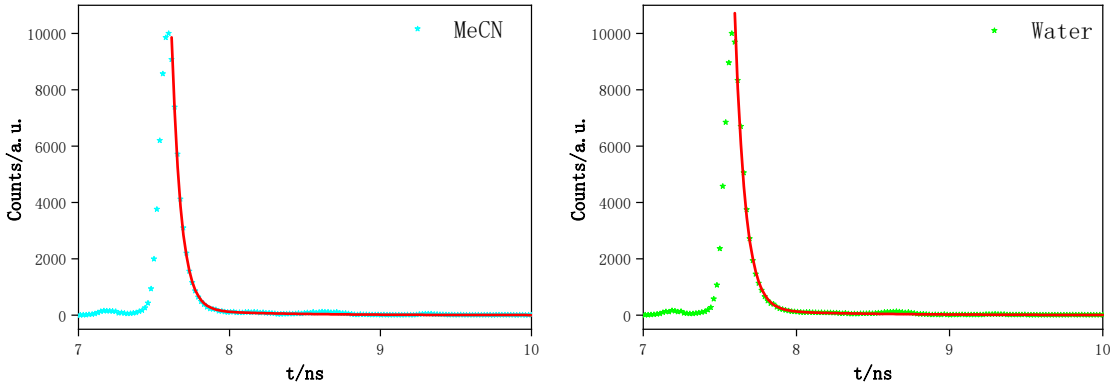



Figure 7. Fluorescence lifetime decay curves of **4g** in polarity solvents

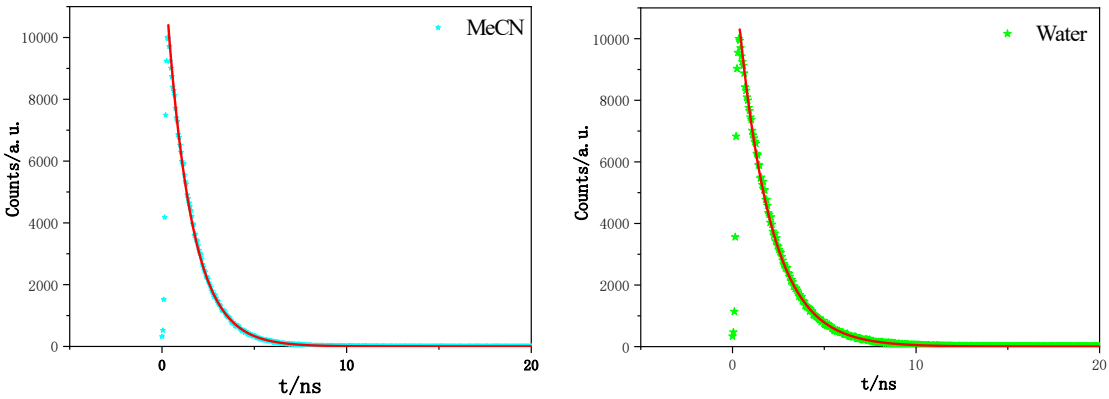



Figure 8. Fluorescence lifetime decay curves of **4h** in polarity solvents

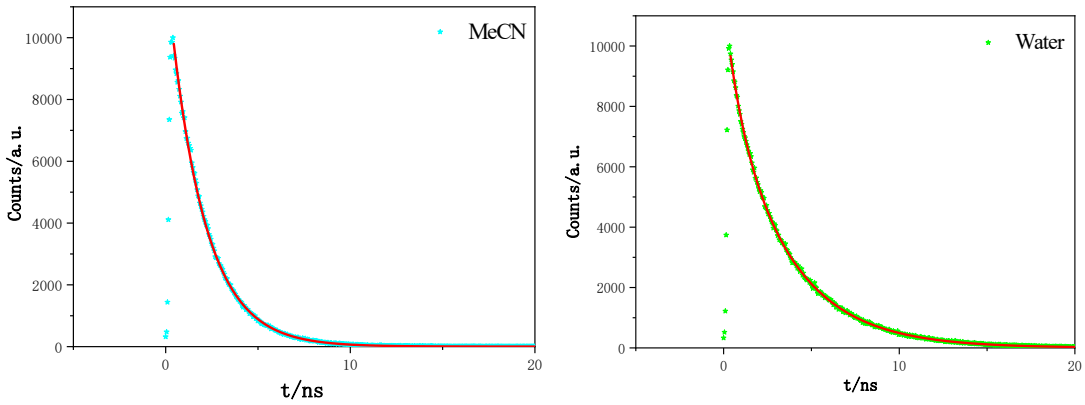
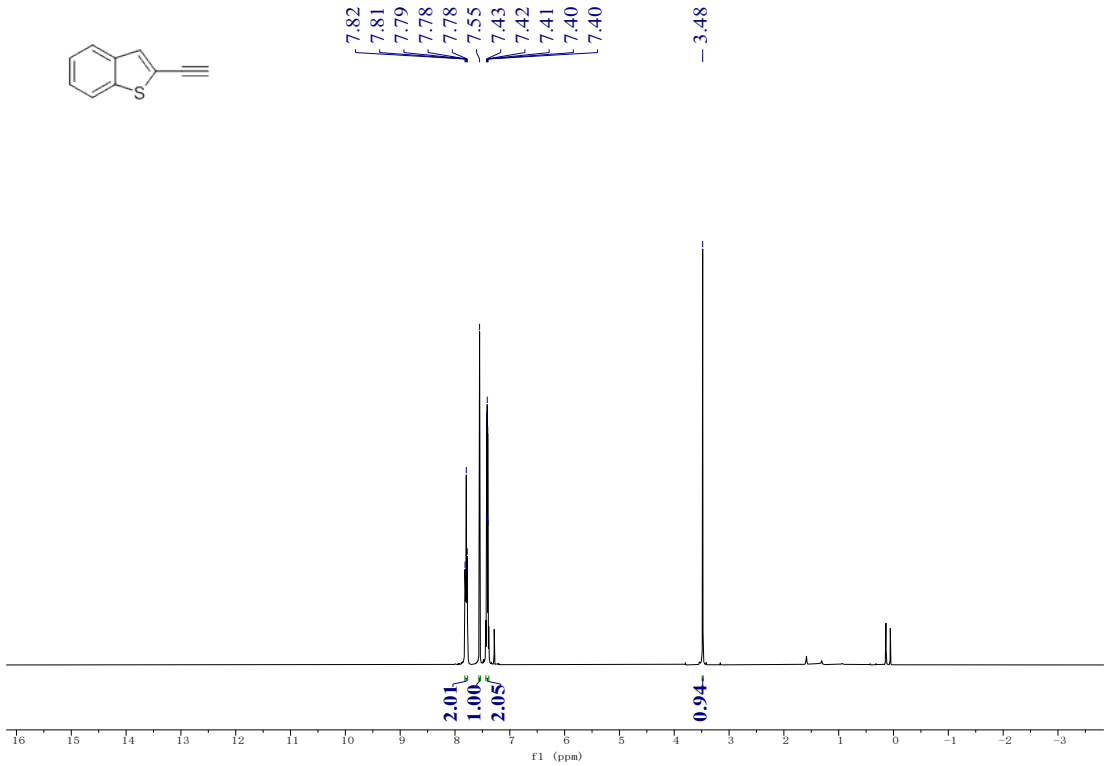


Figure 9. Fluorescence lifetime decay curves of **4i** in polarity solvents

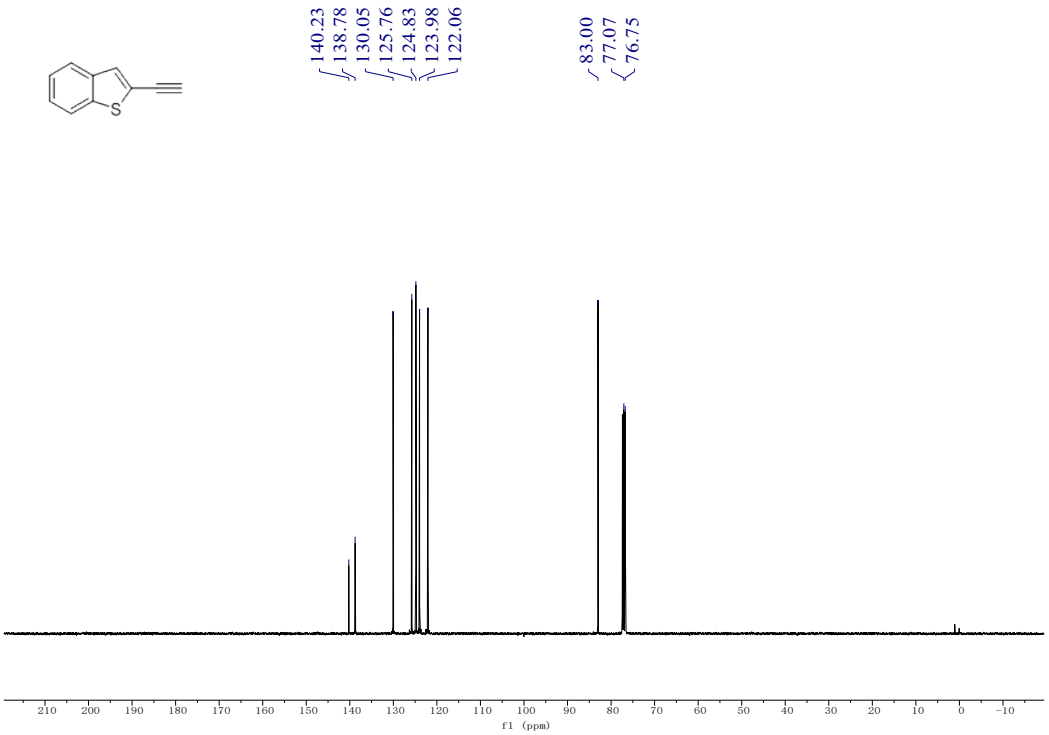
## 5. $^{1}$H NMR, $^{13}$C NMR of compounds

### $^{1}$H NMR Spectrum of Compound 2a



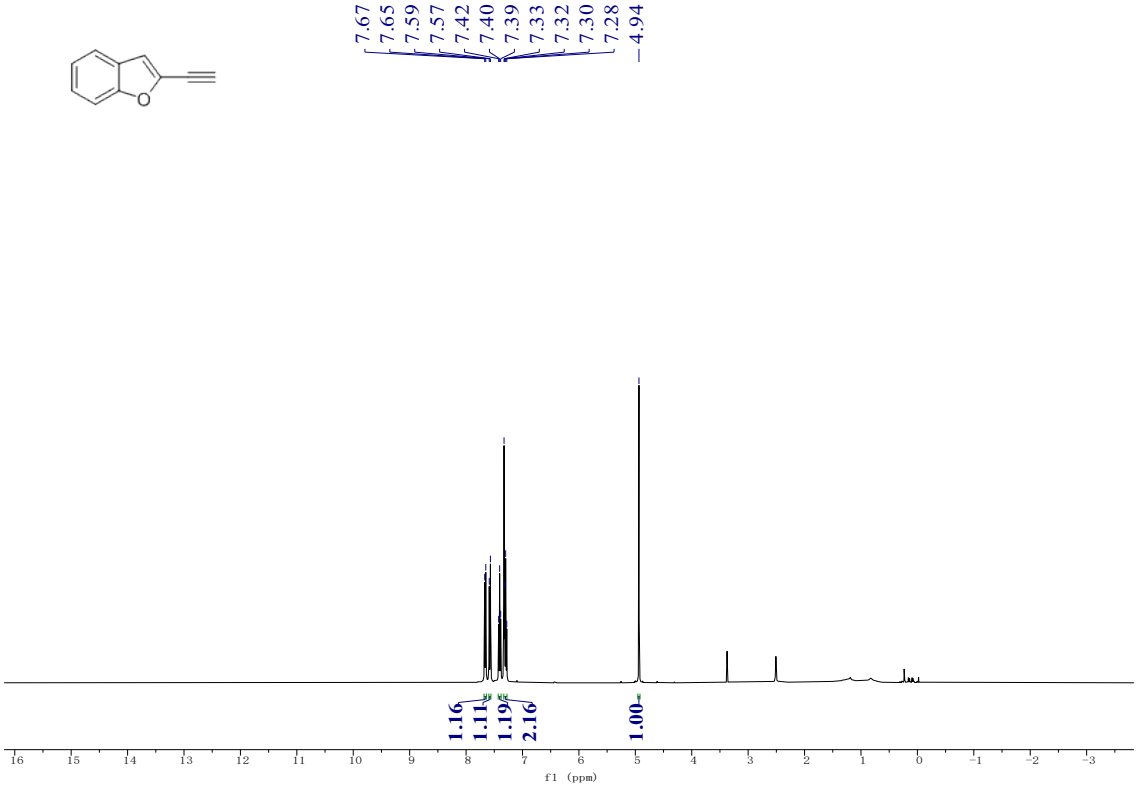

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.83-7.77 (m, 2H), 7.55 (s, 1H), 7.41 (dd, $J$ = 7.3, 3.7 Hz, 2H), 3.48 (s, 1H).

### $^{13}$C NMR Spectrum of Compound 2a



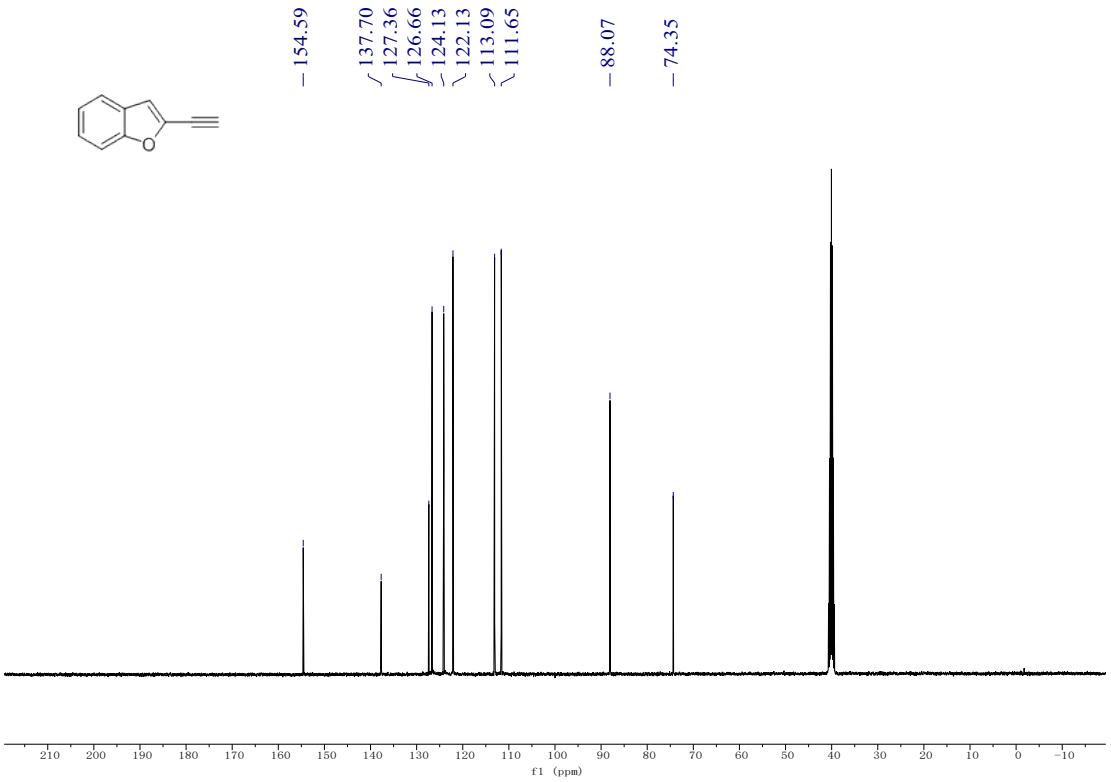

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 140.2, 138.8, 130.1, 125.8, 124.8, 124.0, 122.1, 83.0,77.07,76.75.

## $^{1}$H NMR Spectrum of Compound 2b



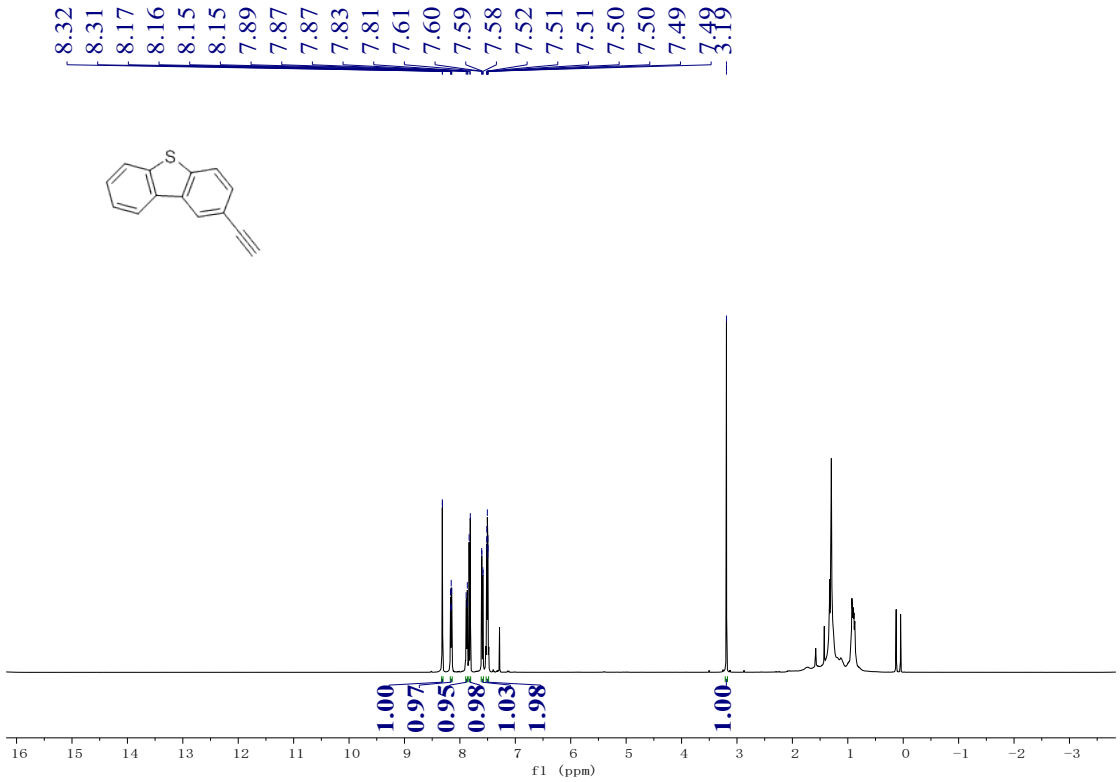

$^{1}$H NMR (400 MHz, DMSO): $\delta$ 7.66 (d, $J$ = 7.7 Hz, 1H), 7.58 (d, $J$ = 8.3 Hz, 1H), 7.40 (t, $J$ = 7.2 Hz, 1H), 7.30 (dd, $J$ = 13.3, 6.1 Hz, 2H), 4.94 (s, 1H).

## $^{13}$C NMR Spectrum of Compound 2b



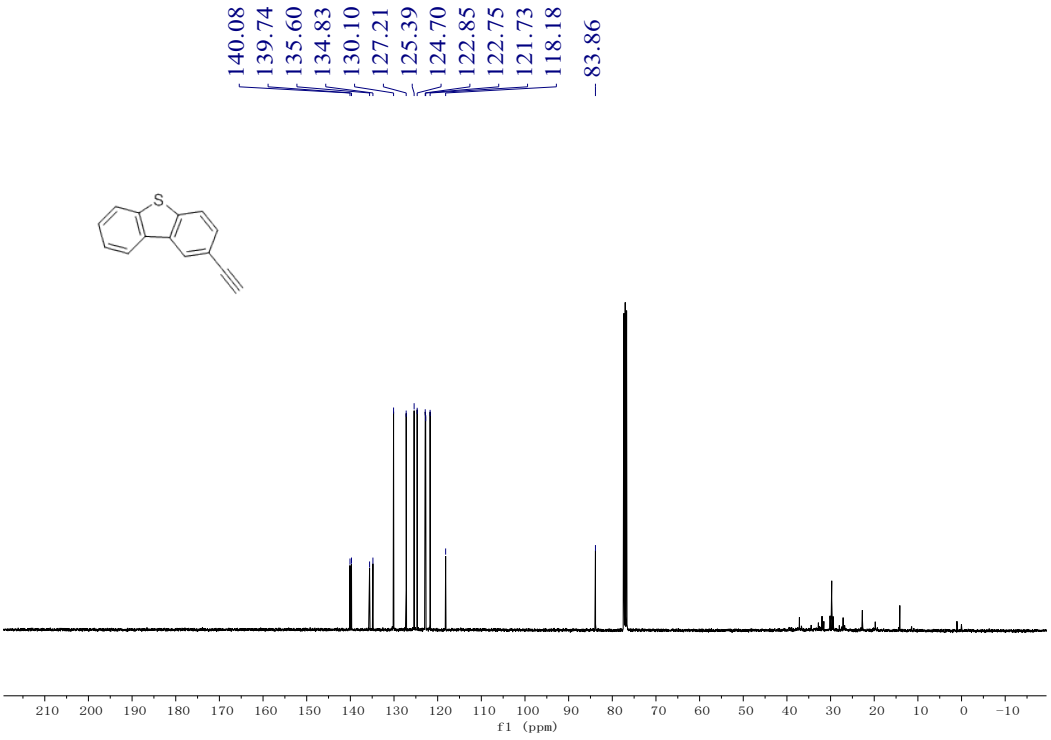

$^{13}$C NMR (101 MHz, DMSO): $\delta$ 154.6, 137.7, 127.4, 126.7, 124.1, 122.1, 113.1, 111.65, 88.1, 74.3.

## $^{1}$H NMR Spectrum of Compound 2c



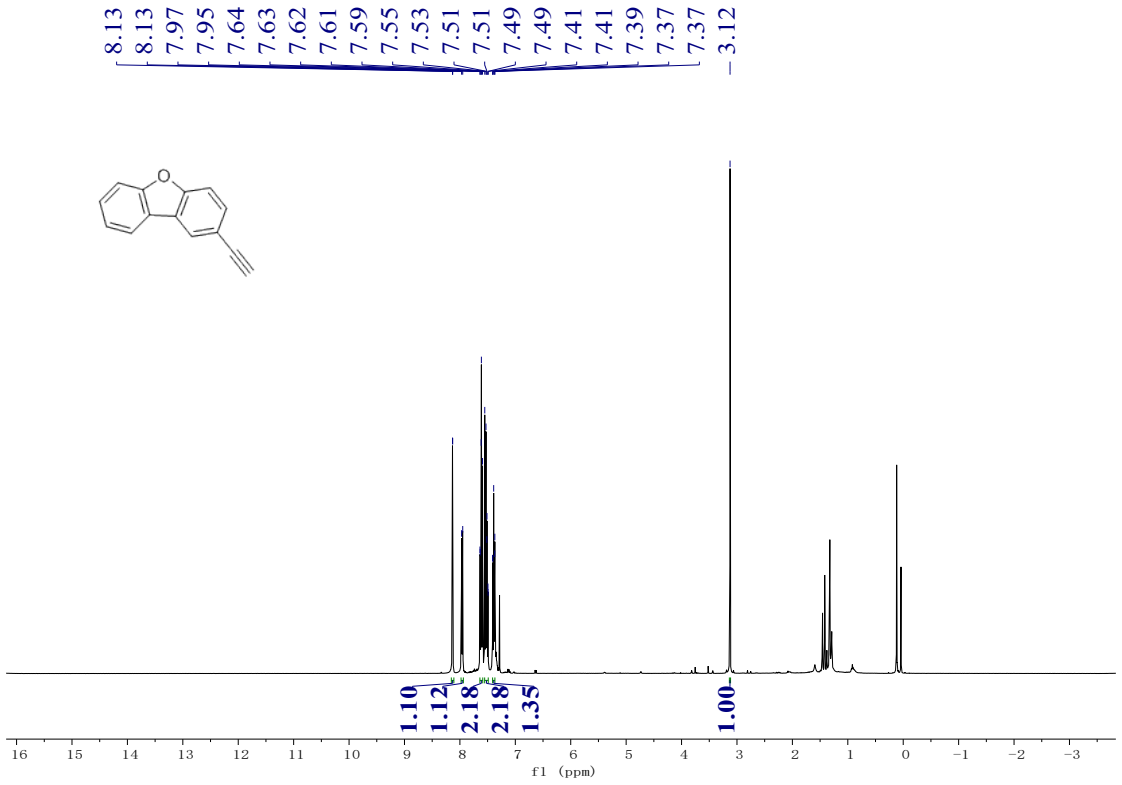

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.32 (d, $J$ = 1.1 Hz, 1H), 8.17-8.14 (m, 1H), 7.89-7.86 (m, 1H), 7.82 (d, $J$ = 8.6 Hz, 1H), 7.59 (dd, $J$ = 8.3, 1.5 Hz, 1H), 7.53-7.48 (m, 2H), 3.19 (s, 1H).

## $^{13}$C NMR Spectrum of Compound 2c



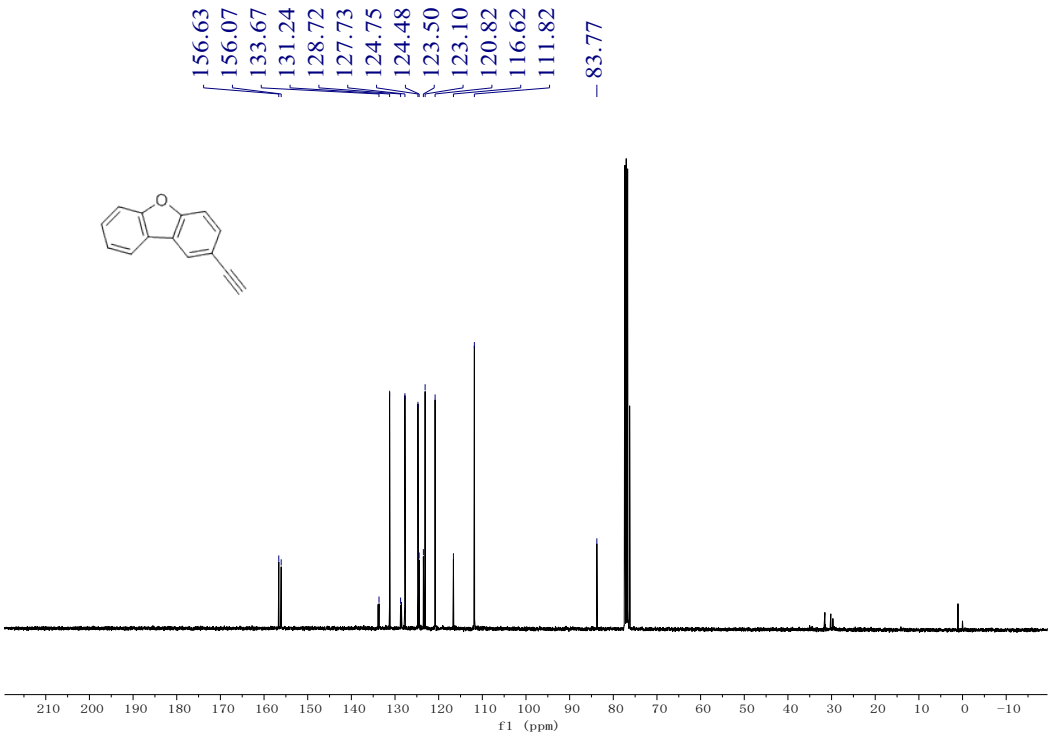

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 140.1, 139.7, 135.6, 134.8, 130.1, 127.2, 125.4, 124.7, 122.8, 122.7, 121.7, 118.2, 83.9.

## $^{1}$H NMR Spectrum of Compound 2d



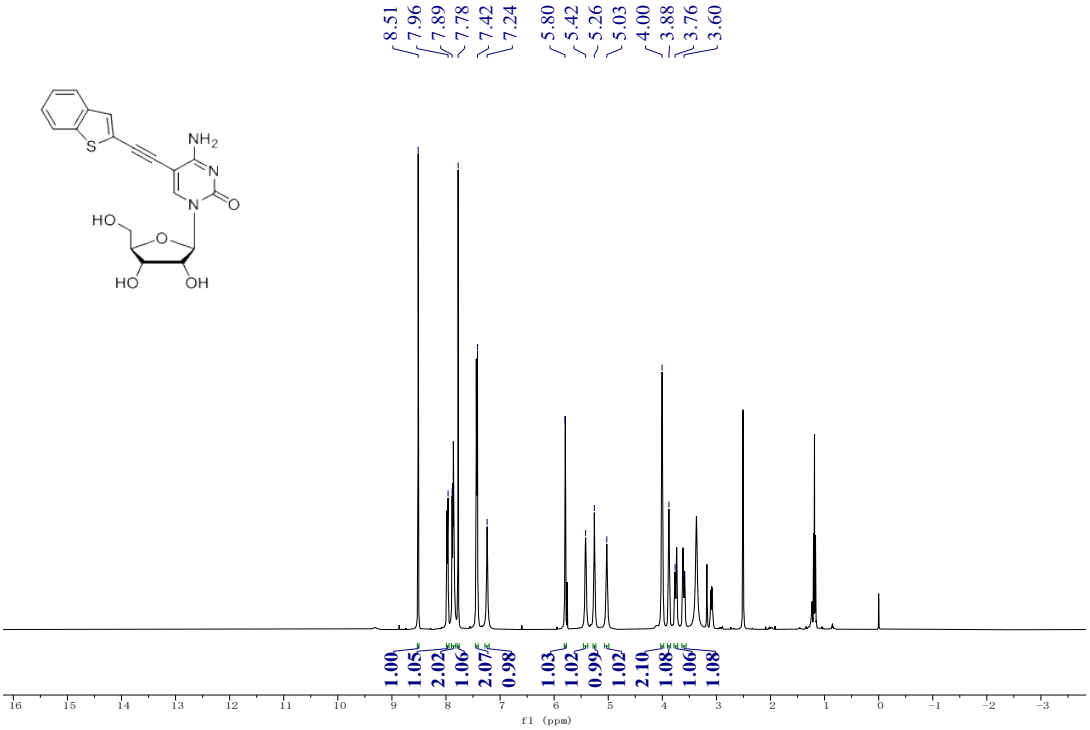

$^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ 8.13 (d, $J$ = 1.3 Hz, 1H), 7.96 (d, $J$ = 8.2 Hz, 1H), 7.64-7.59 (m, 2H), 7.55-7.49 (m, 2H), 7.41-7.37 (m, 1H), 3.12 (s, 1H).

## $^{13}$C NMR Spectrum of Compound 2d



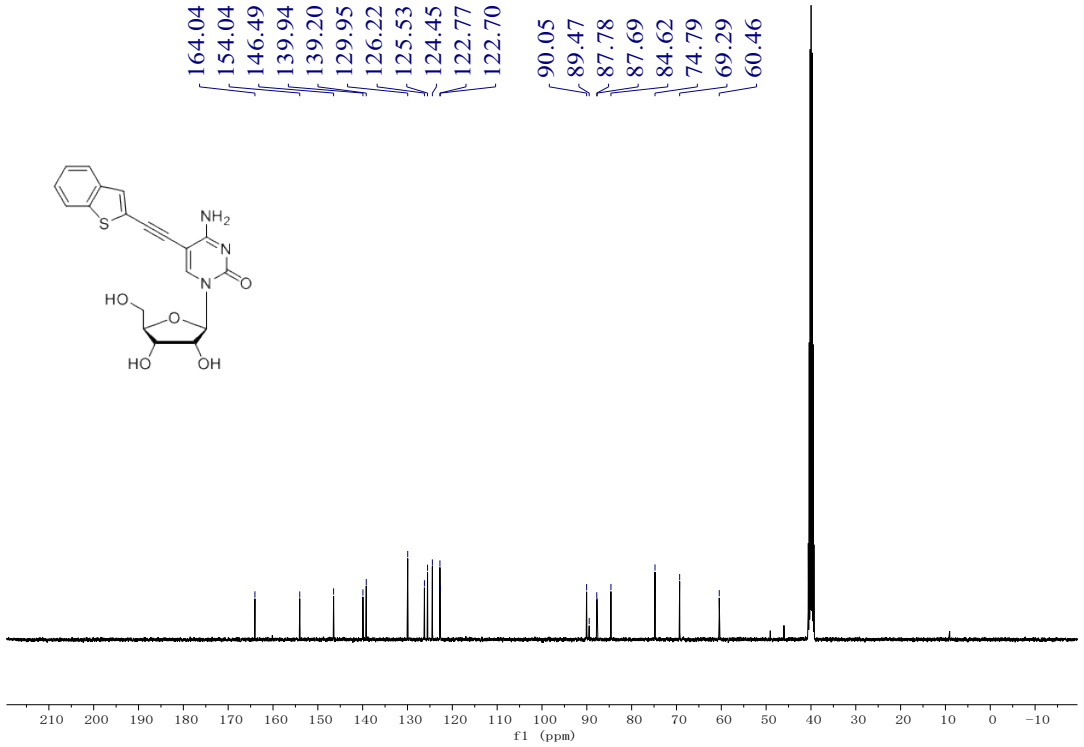

$^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ 156.6, 156.1, 133.7, 131.2, 128.7, 127.7, 124.7, 124.5, 123.5, 123.1, 120.8, 116.6, 111.8, 83.8.

## $^{1}$H NMR Spectrum of Compound 3a



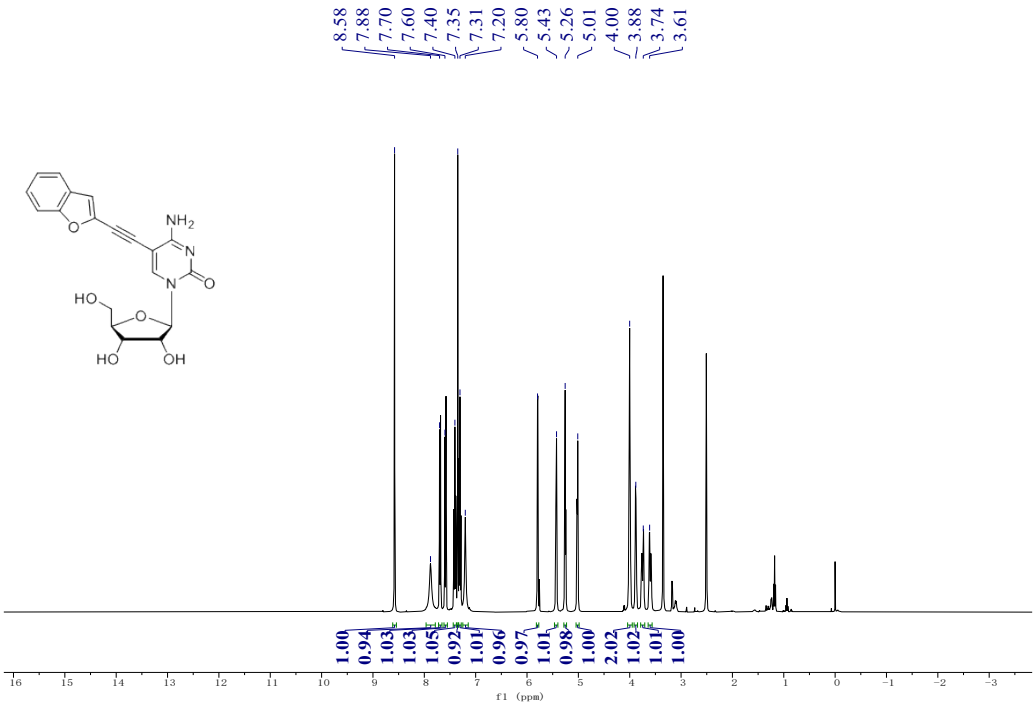

$^{1}$H NMR (400 MHz, DMSO): $\delta$ 8.51 (s, 1H), 7.99-7.94 (m, 1H), 7.89 (dd, $J$ = 6.2, 2.9 Hz, 2H), 7.78 (s, 1H), 7.46-7.40 (m, 2H), 7.24 (s, 1H), 5.80 (d, $J$ = 2.8 Hz, 1H), 5.42 (s, 1H), 5.26 (s, 1H), 5.03 (s, 1H), 4.00 (s, 2H), 3.88 (d, $J$ = 2.5 Hz, 1H), 3.76 (d, $J$ = 12.0 Hz, 1H), 3.60 (d, $J$ = 8.7 Hz, 1H).

## $^{13}$C NMR Spectrum of Compound 3a



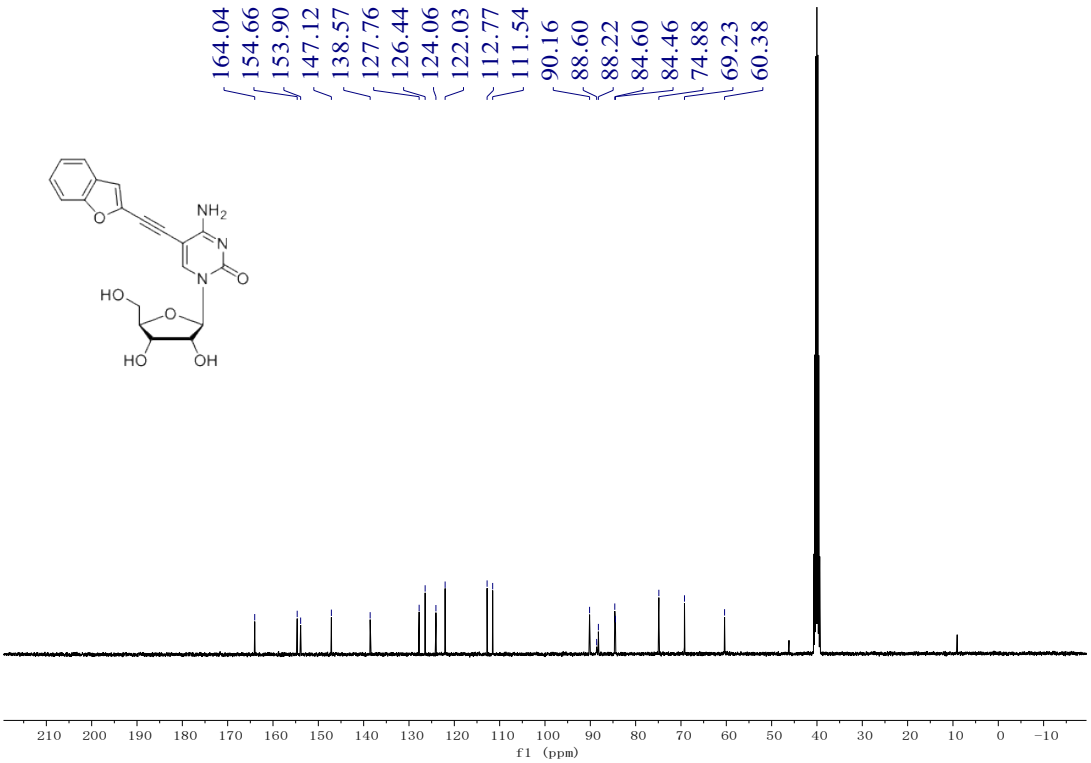

$^{13}$C NMR (101 MHz, DMSO): $\delta$ 164.0, 154.0, 146.5, 139.9, 139.2, 130.0, 126.2, 125.5, 124.5, 122.8, 122.7, 90.0, 89.5, 87.8, 87.7, 84.6, 74.8, 69.3, 60.5.

## $^{1}$H NMR Spectrum of Compound 3b



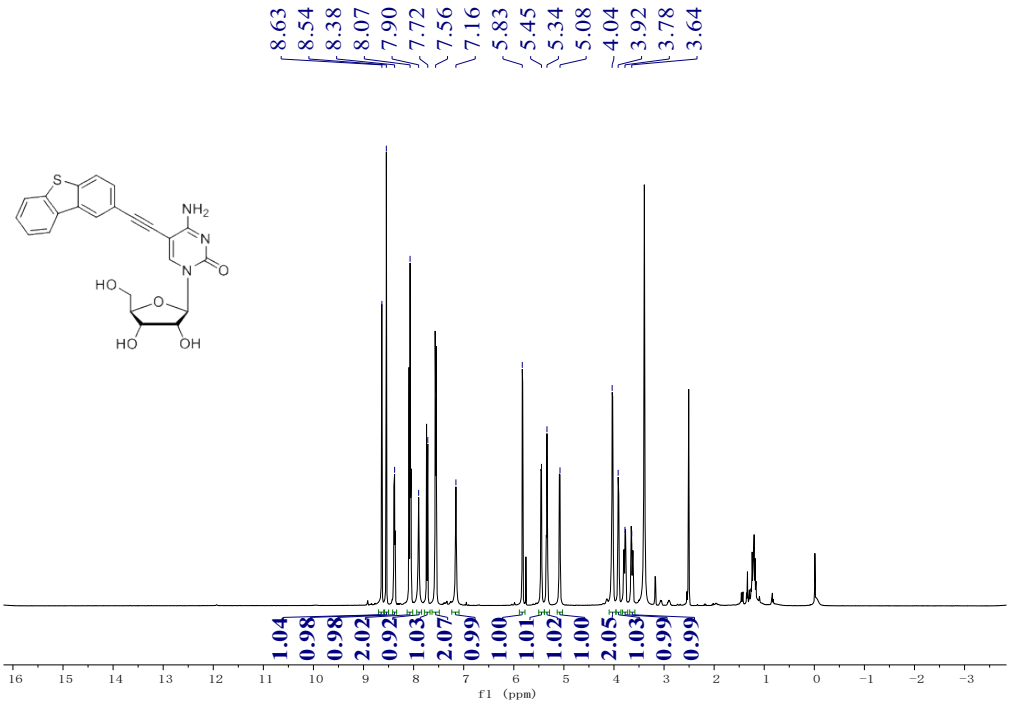

$^{1}$H NMR (400 MHz, DMSO): $\delta$ 8.58 (s, 1H), 7.88 (s, 1H), 7.70 (d, $J$ = 7.5 Hz, 1H), 7.60 (d, $J$ = 8.3 Hz, 1H), 7.40 (t, $J$ = 7.7 Hz, 1H), 7.35 (d, $J$ = 0.7 Hz, 1H), 7.31 (t, $J$ = 7.5 Hz, 1H),7.20(s, 1H), 5.80 (d, $J$ = 2.6 Hz, 1H), 5.43 (d, $J$ = 4.5 Hz, 1H), 5.26 (t, $J$ = 4.8 Hz, 1H), 5.01 (d, $J$ = 5.2 Hz, 1H), 4.00 (s, 2H), 3.92-3.85 (m, 1H), 3.79-3.71 (m, 1H), 3.64-3.56 (m, 1H).

## $^{13}$C NMR Spectrum of Compound 3b



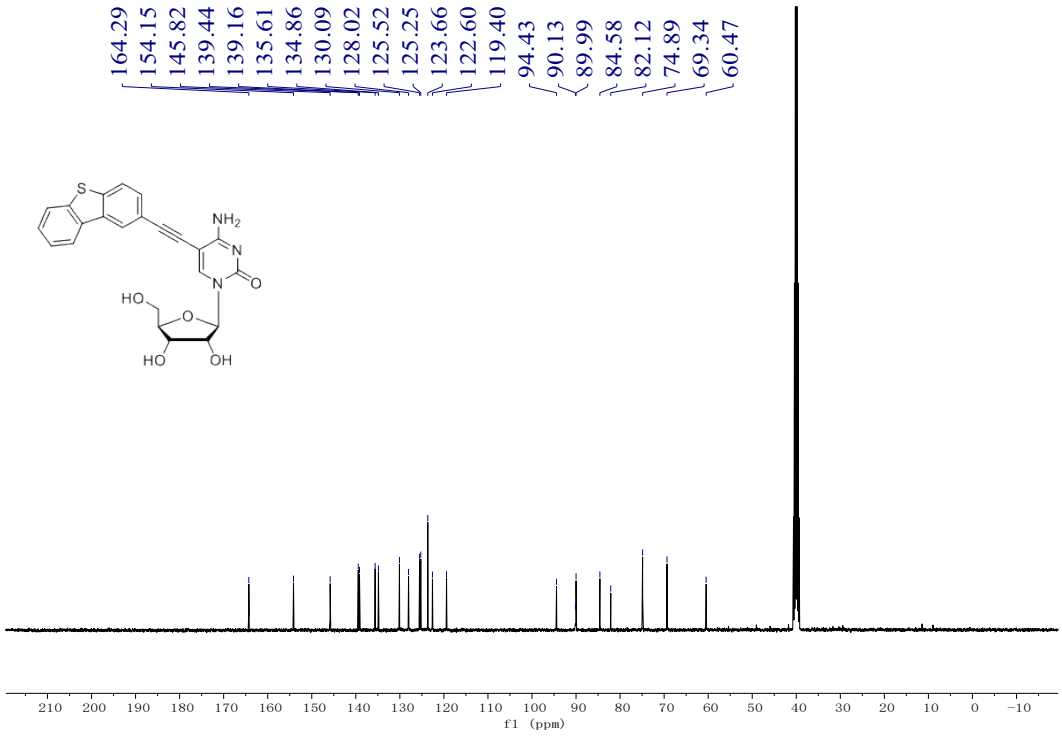

$^{13}$C NMR (101 MHz, DMSO): $\delta$ 164.0, 154.7, 153.9, 147.1, 138.6, 127.8, 126.4, 124.1, 122.0, 112.8, 111.5, 90.2, 88.6, 88.2, 84.6, 84.5, 74.9, 69.2, 60.4.

## $^{1}$H NMR Spectrum of Compound 3c



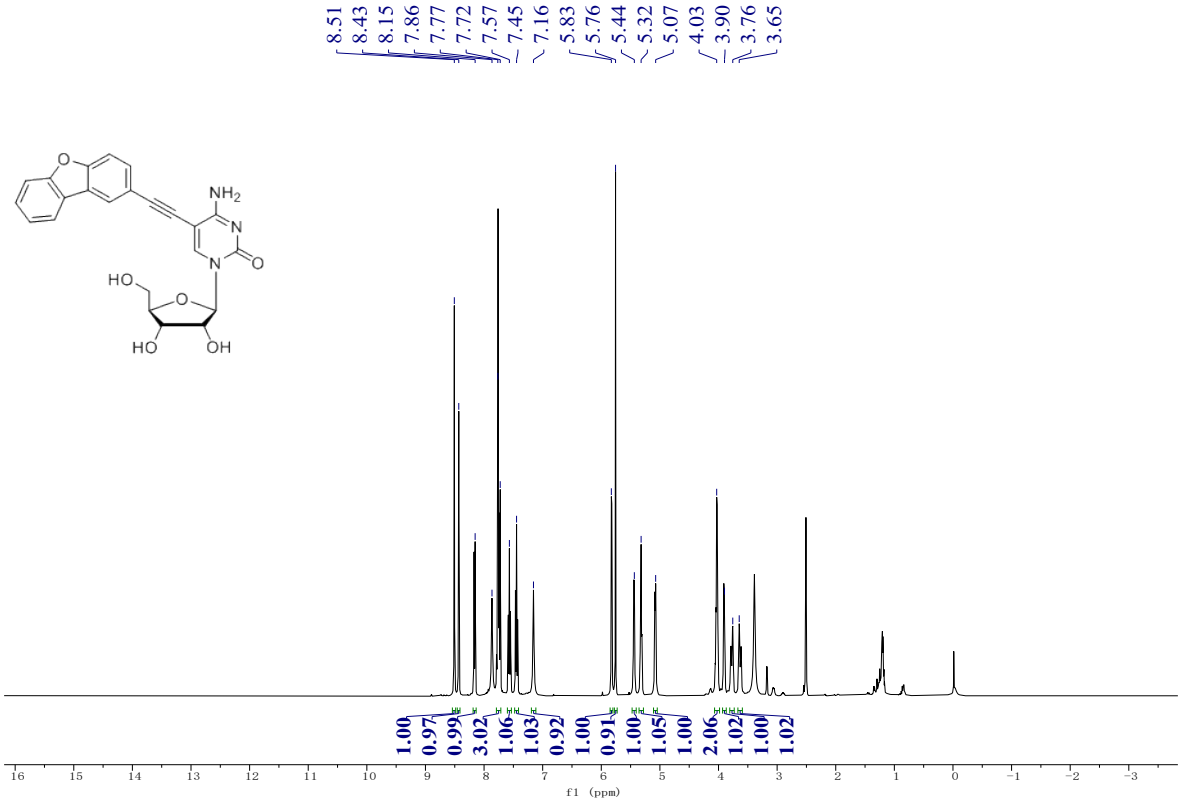

$^{1}$H NMR (400 MHz, DMSO): $\delta$ 8.63 (d, $J$ = 1.0 Hz, 1H), 8.54 (s, 1H), 8.38 (dd, $J$ = 6.3, 2.8 Hz, 1H), 8.13-8.02 (m, 2H), 7.90 (s, 1H), 7.72 (dd, $J$ = 8.3, 1.5 Hz, 1H), 7.63-7.49 (m, 2H), 7.16 (s, 1H), 5.83 (s, 1H), 5.45 (s, 1H), 5.34 (s, 1H), 5.08 (s, 1H), 4.04 (dd, $J$ = 8.4, 4.4 Hz, 2H), 3.96-3.86 (m, 1H), 3.83-3.73 (m, 1H), 3.69-3.58 (m, 1H).

## $^{13}$C NMR Spectrum of Compound 3c



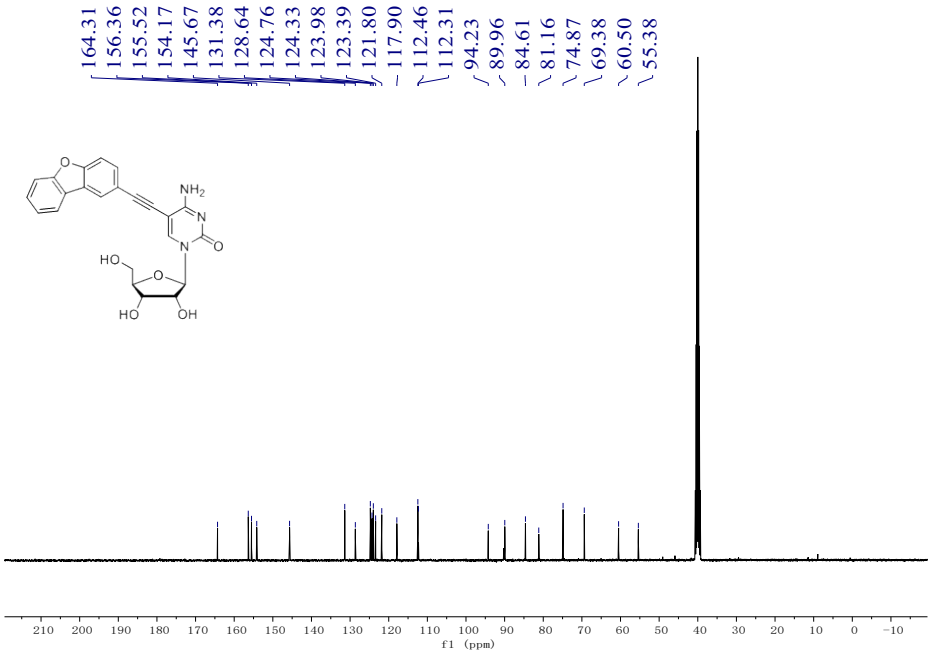

$^{13}$C NMR (101 MHz, DMSO): $\delta$ 164.3, 154.1, 145.8, 139.4, 139.2, 135.6, 134.9, 130.1, 128.0, 125.5, 125.3, 123.7, 122.6, 119.4, 94.4, 90.1, 90.0, 84.6, 82.1, 74.9, 69.3, 60.5.

## $^{1}$H NMR Spectrum of Compound 3d.



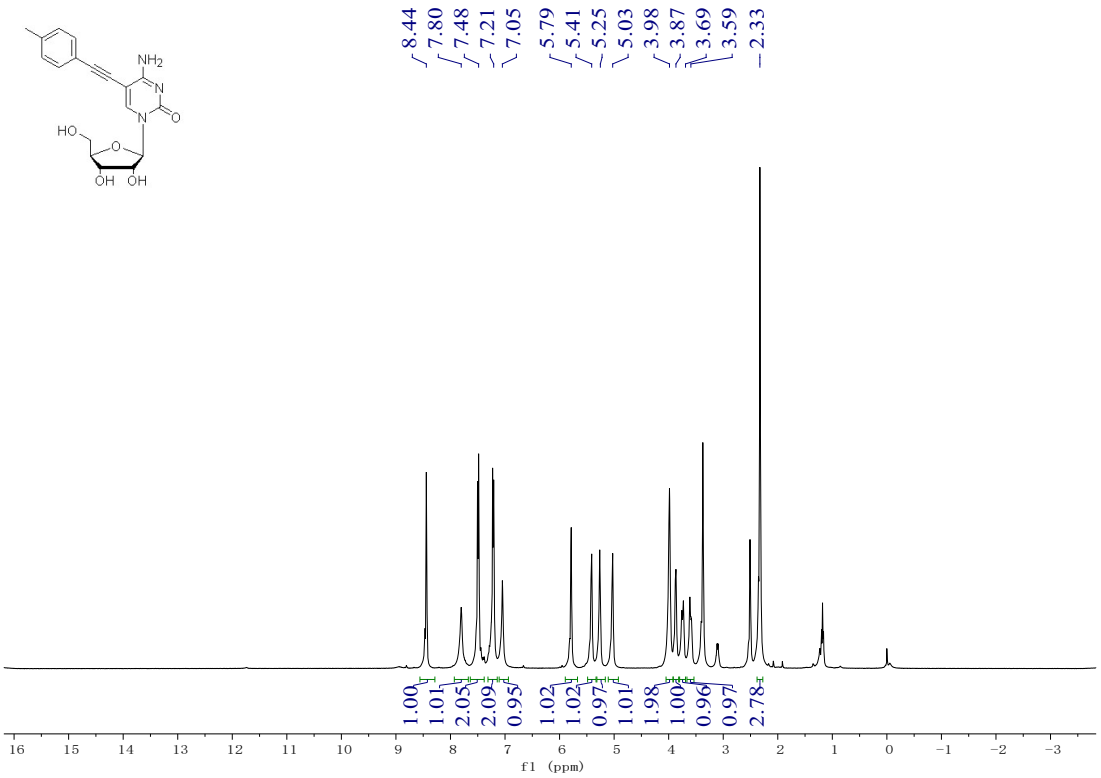

$^{1}$H NMR (400 MHz, DMSO): $\delta$ 8.51 (s, 1H), 8.43 (s, 1H), 8.15 (d, $J$ = 7.4 Hz, 1H), 7.86-7.71 (m, 3H), 7.60-7.53 (m, 1H), 7.45 (t, $J$ = 7.5 Hz, 1H), 7.16 (s, 1H), 5.83 (d, $J$ = 3.1 Hz, 1H), 5.76 (s, 1H), 5.44 (d, $J$ = 4.3 Hz, 1H), 5.32 (t, $J$ = 4.7 Hz, 1H), 5.07 (d, $J$ = 4.8 Hz, 1H), 4.03 (d, $J$ = 3.1 Hz, 2H), 3.93-3.87 (m, 1H), 3.81-3.73 (m, 1H), 3.67-3.59 (m, 1H).

## $^{13}$C NMR Spectrum of Compound 3d



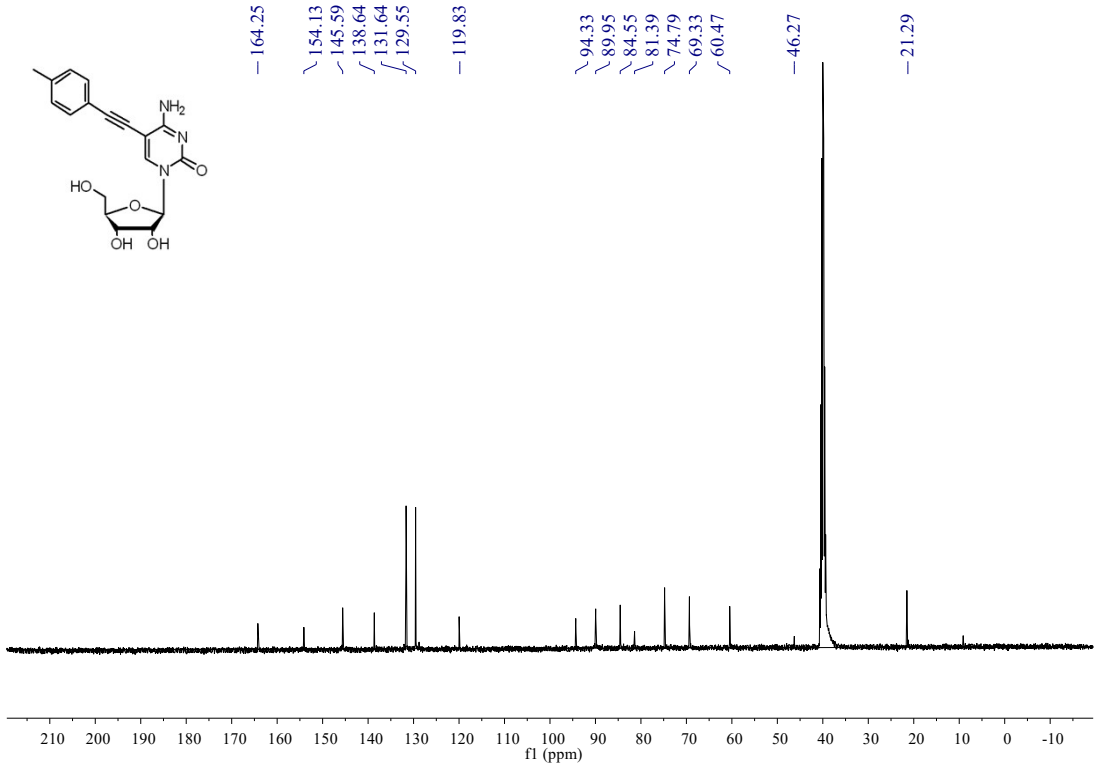

$^{13}$C NMR (101 MHz, DMSO): $\delta$ 164.3, 156.4, 155.5, 154.2, 145.7, 131.4, 128.6, 124.8, 124.3, 124.0, 123.4, 121.8, 117.9, 112.5, 112.3, 94.2, 90.0, 84.6, 81.2, 74.9, 69.4, 60.5, 55.4.

## $^{1}$H NMR Spectrum of Compound 3e



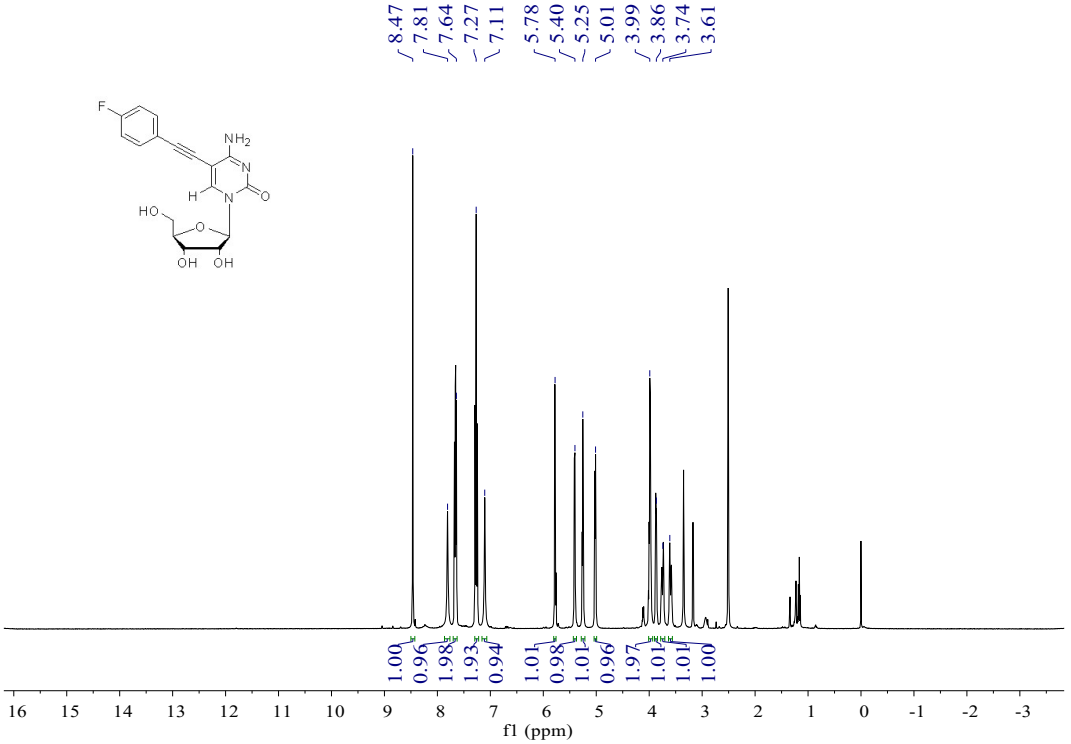

$^{1}$H NMR (400 MHz, DMSO-*d6*) 8.44 (s, 1H), 7.80 (s, 1H),7.48 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.05 (s, 1H), 5.79 (s, 1H), 5.41 (s, 1H), 5.25 (s, 1H), 5.03 (s, 1H), 3.98 (s, 2H), 3.87 (s, 1H), 3.69 (s, 1H), 3.59 (s, 1H), 2.33 (s, 3H).

## $^{13}$C NMR Spectrum of Compound 3e



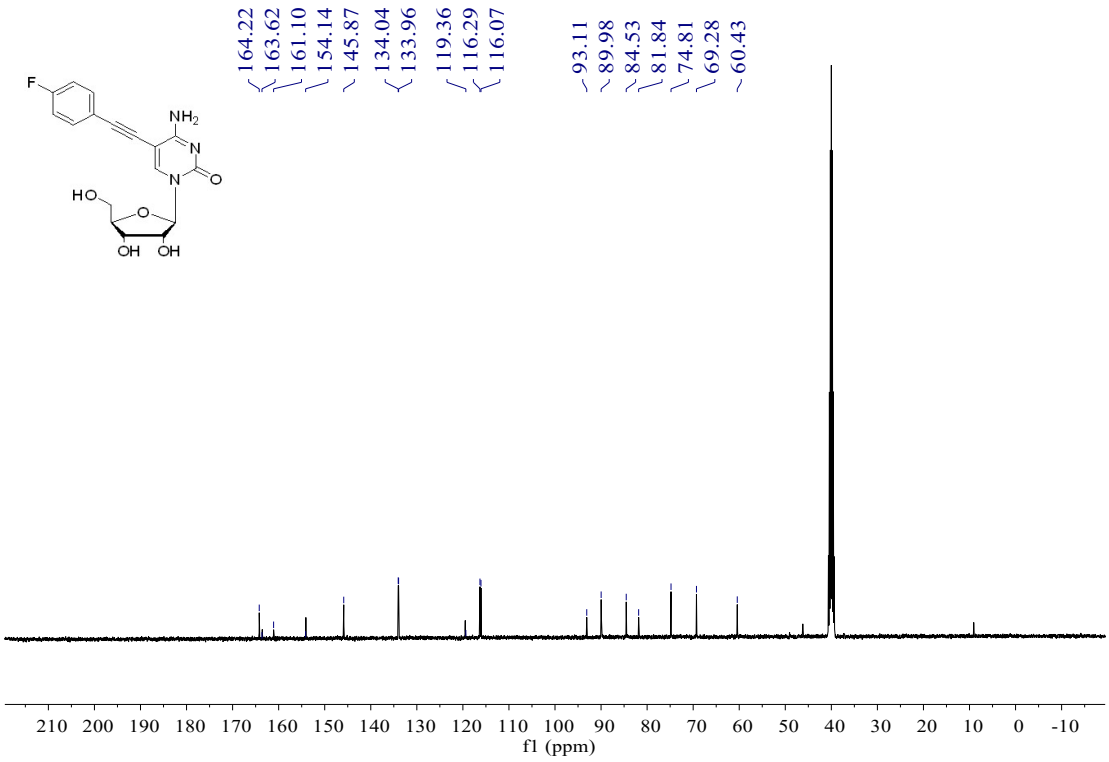

$^{13}$C NMR (101 MHz, DMSO-*d6*) $\delta$ 164.3, 154.1, 145.6, 138.6, 131.6, 129.6, 119.8, 94.3, 90.0, 84.6, 81.4, 74.8, 69.3, 60.5, 21.3.

## $^{1}$H NMR Spectrum of Compound 3f



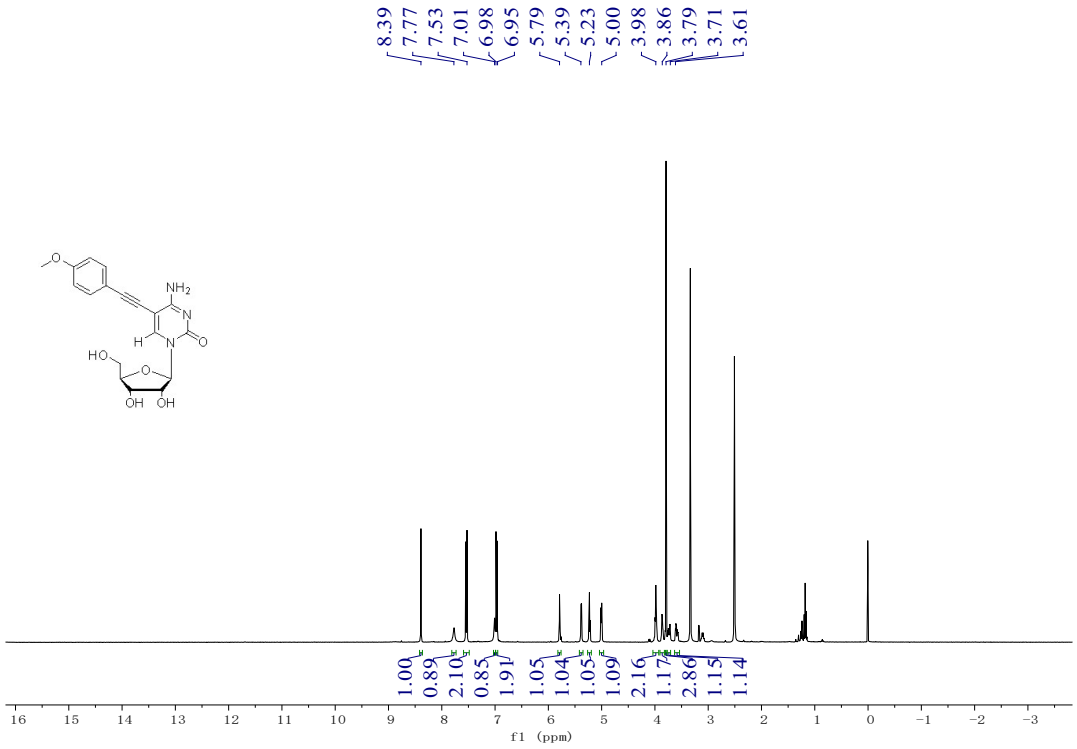

$^{1}$H NMR (400 MHz, DMSO-*d6*) $\delta$ 8.47 (s, 1H), 7.81 (s, 1H), 7.64 (s, 2H), 7.27 (t, $J$ = 8.9 Hz, 2H), 7.11 (s, 1H), 5.78 (d, $J$ = 3.0 Hz, 1H), 5.40 (d, $J$ = 4.6 Hz, 1H), 5.25 (t, $J$ = 4.7 Hz, 1H), 5.01 (d, $J$ = 5.2 Hz, 1H), 3.99 (s, 2H), 3.86 (s, 1H), 3.74 (s, 1H), 3.61 (s, 1H).

## $^{13}$C NMR Spectrum of Compound 3f



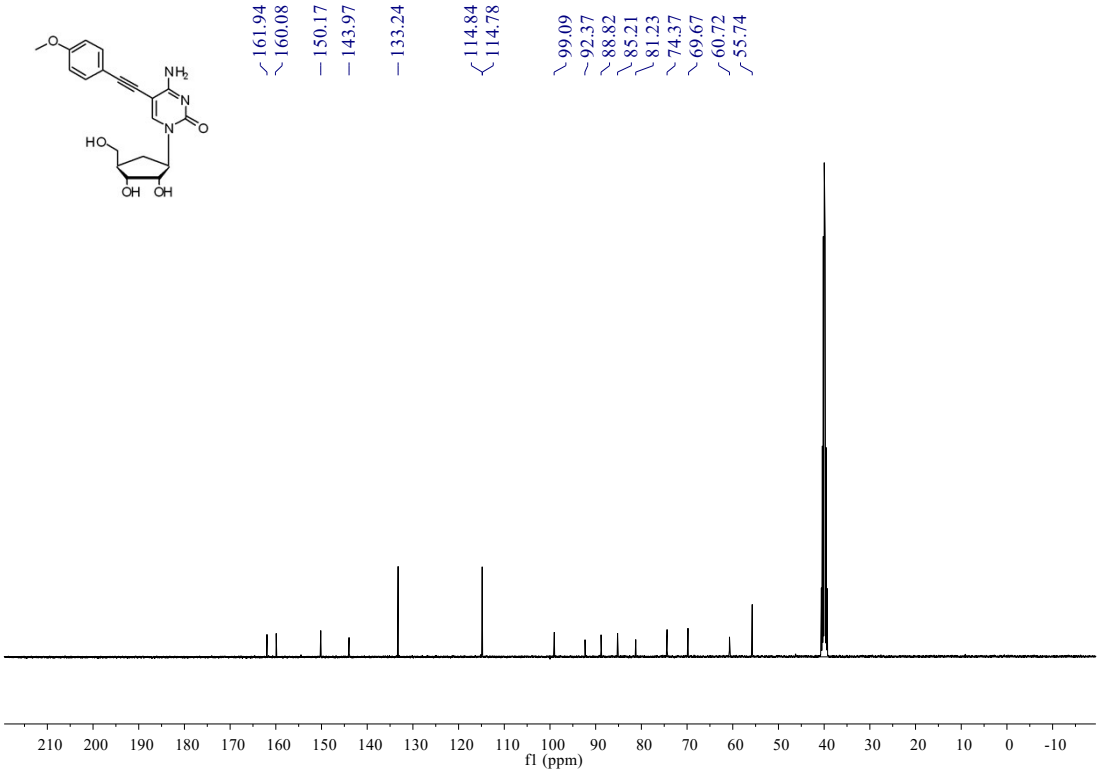

$^{13}$C NMR (101 MHz, DMSO-*d6*) $\delta$ 164.2, 163.6, 154.1, 145.9, 134.0, 140.0,119.4, 116.3, 116.1, 93.1, 90.0, 84.5, 81.8, 74.8, 69.3, 60.4.

## $^{1}$H NMR Spectrum of Compound 3g



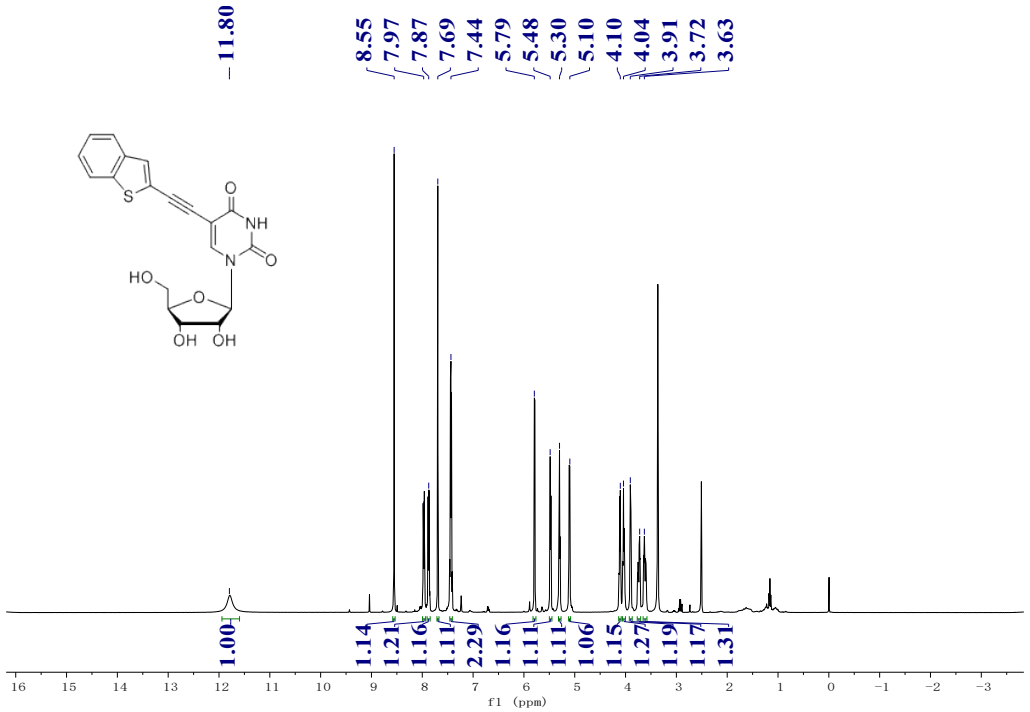

$^{1}$H NMR (400 MHz, DMSO-*d6*) $\delta$ 8.39 (s, 1H), 7.77 (s, 1H), 7.53 (d, $J$ = 11.5 Hz, 2H), 7.01 (s, 1H), 6.98 (s, 1H), 6.95 (s, 1H), 5.79 (s, 1H), 5.39 (s, 1H), 5.23 (s, 1H), 5.00 (s, 1H), 3.98 (s, 2H), 3.89-3.84 (m, 1H), 3.79 (s, 3H), 3.71 (s, 1H), 3.61 (s, 1H).

## $^{13}$C NMR Spectrum of Compound 3g



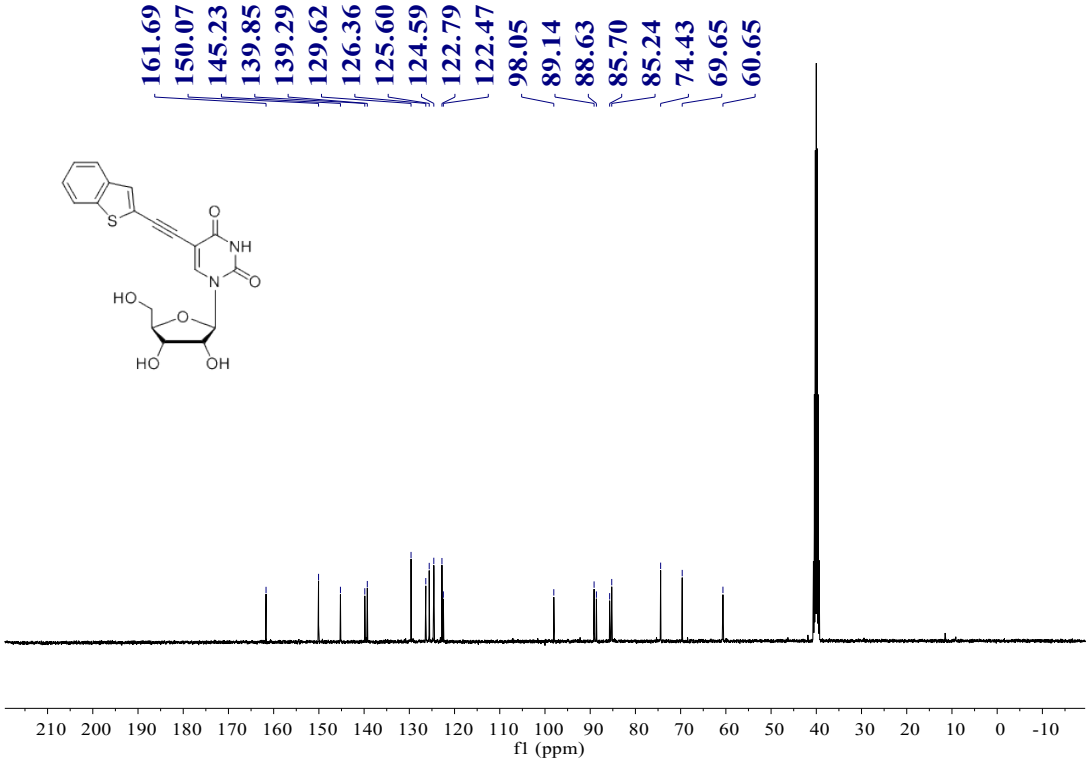

$^{13}$C NMR (101 MHz, DMSO-*d6*) $\delta$ 161.9, 160.1, 150.2, 144.0, 133.2, 114.8, 114.8, 99.1, 92.4, 88.8, 85.2, 81.2, 74.4, 69.7, 60.7, 55.7.

## $^{1}$H NMR Spectrum of Compound 3h



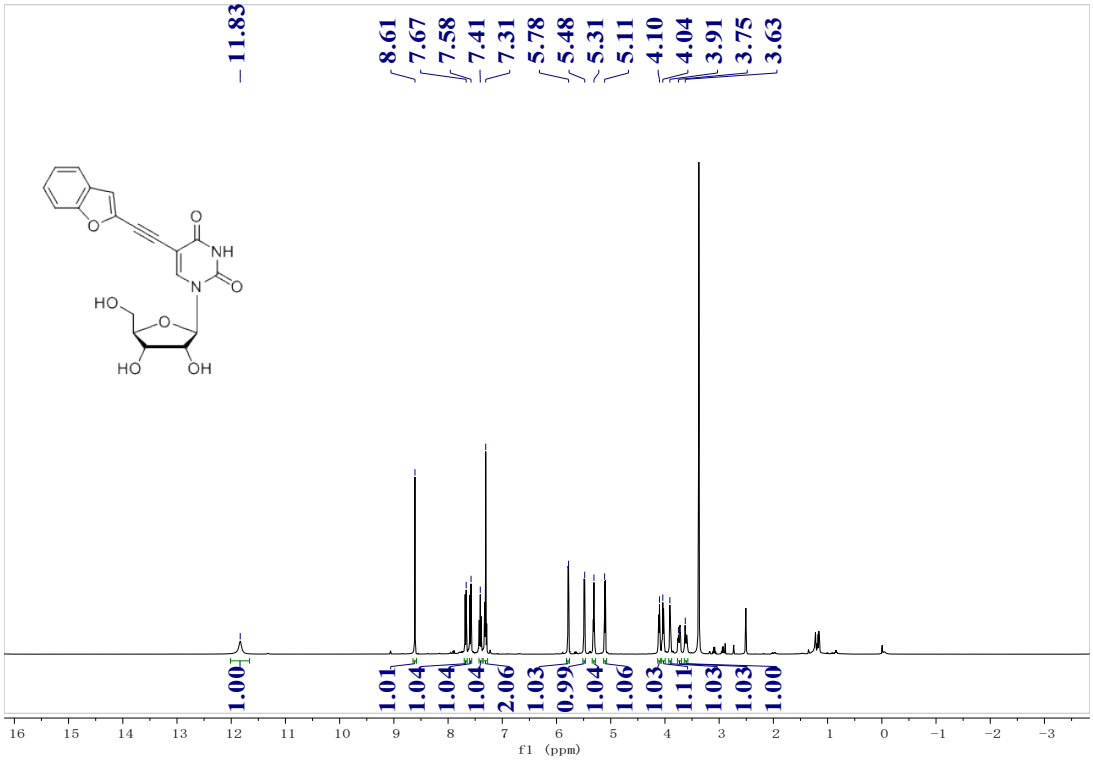

$^{1}$H NMR (400 MHz, DMSO): $\delta$ 11.80 (s, 1H), 8.55 (s, 1H), 7.99-7.93 (m, 1H), 7.90-7.84 (m, 1H), 7.69 (s, 1H), 7.46-7.41 (m, 2H), 5.79 (d, $J$ = 4.4 Hz, 1H), 5.48 (d, $J$ = 5.3 Hz, 1H), 5.30 (t, $J$ = 4.8 Hz, 1H), 5.10 (d, $J$ = 5.5 Hz, 1H), 4.10 (dd, $J$ = 9.6, 4.8 Hz, 1H), 4.04 (dd, $J$ = 10.0, 5.0 Hz, 1H), 3.93-3.87 (m, 1H), 3.72 (dd, $J$ = 9.9, 6.5 Hz, 1H), 3.65-3.58 (m, 1H).

## $^{13}$C NMR Spectrum of Compound 3h



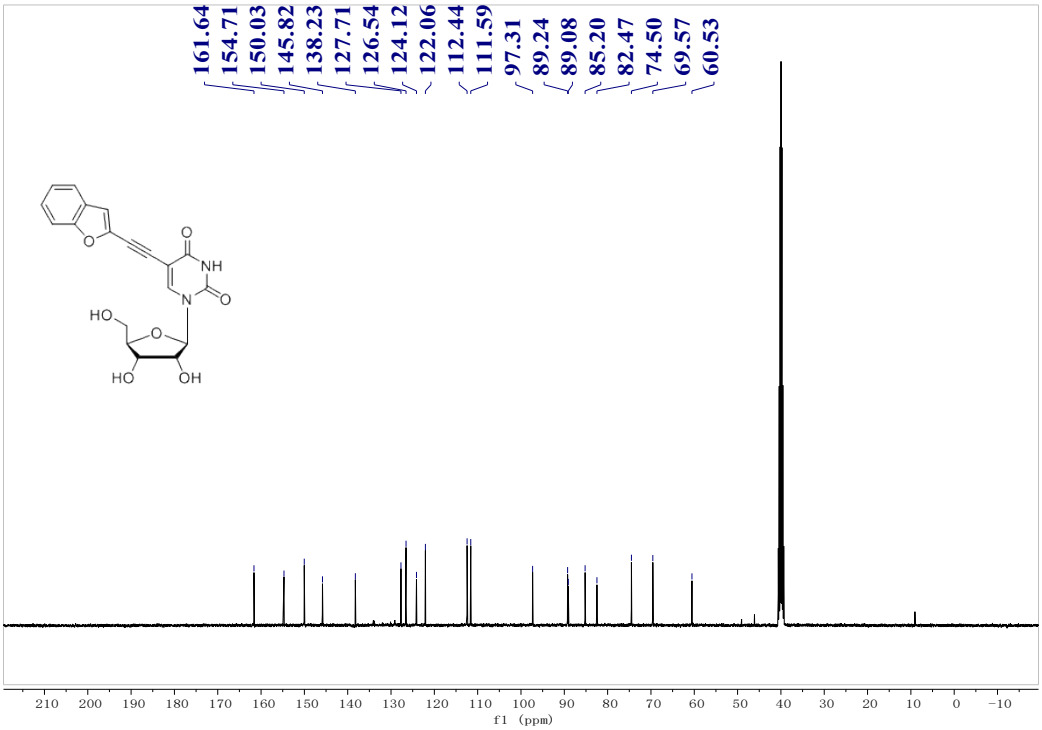

$^{13}$C NMR (101 MHz, DMSO): $\delta$ 161.7, 150.1, 145.2, 139.3, 139.3, 129.6, 126.4, 125.6, 124.6, 122.8, 122.5, 98.1, 89.1, 88.6, 85.7, 85.2, 74.4, 69.7, 60.7.

## $^{1}$H NMR Spectrum of Compound 3i



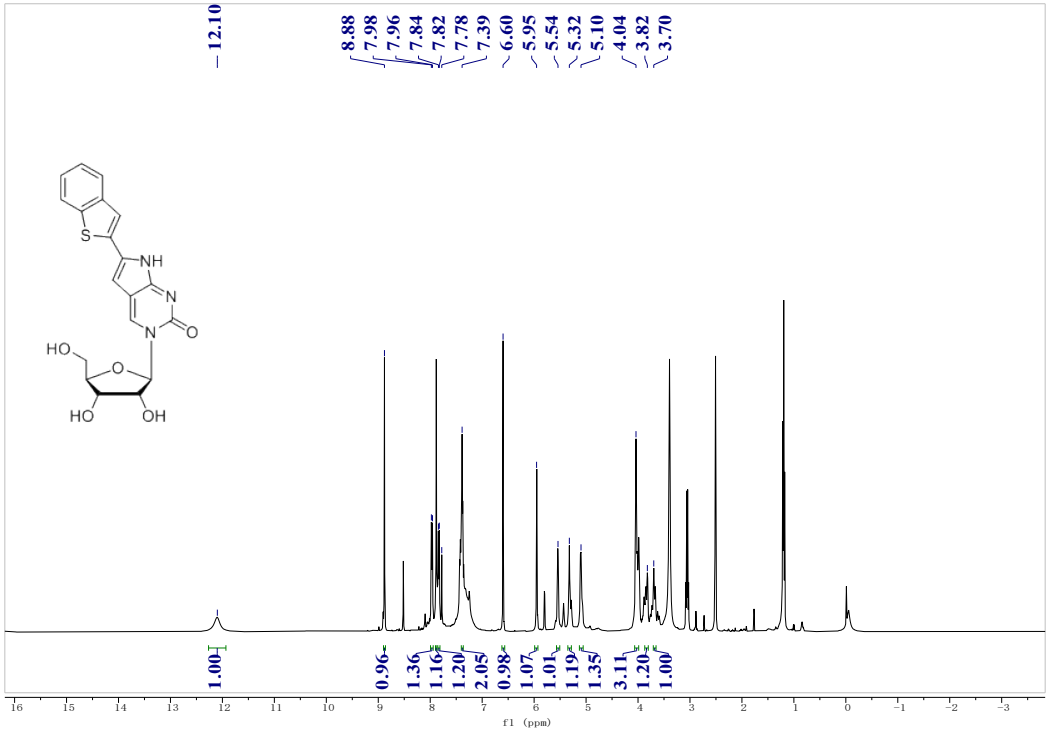

$^{1}$H NMR (400 MHz, DMSO): $\delta$ 11.83 (s, 1H), 8.61 (s, 1H), 7.67 (d, $J$ = 7.7 Hz, 1H), 7.58 (d, $J$ = 8.3 Hz, 1H), 7.43-7.37 (m, 1H), 7.35-7.27 (m, 2H), 5.78 (d, $J$ = 4.3 Hz, 1H), 5.48 (d, $J$ = 5.2 Hz, 1H), 5.31 (t, $J$ = 4.8 Hz, 1H), 5.11 (d, $J$ = 5.5 Hz, 1H), 4.10 (dd, $J$ = 9.6, 4.8 Hz, 1H), 4.04 (dd, $J$ = 10.3, 5.1 Hz, 1H), 3.93-3.88 (m, 1H), 3.75 (ddd, $J$ = 11.8, 4.4, 3.0 Hz, 1H), 3.63 (ddd, $J$ = 12.0, 4.4, 2.8 Hz, 1H).

## $^{13}$C NMR Spectrum of Compound 3i



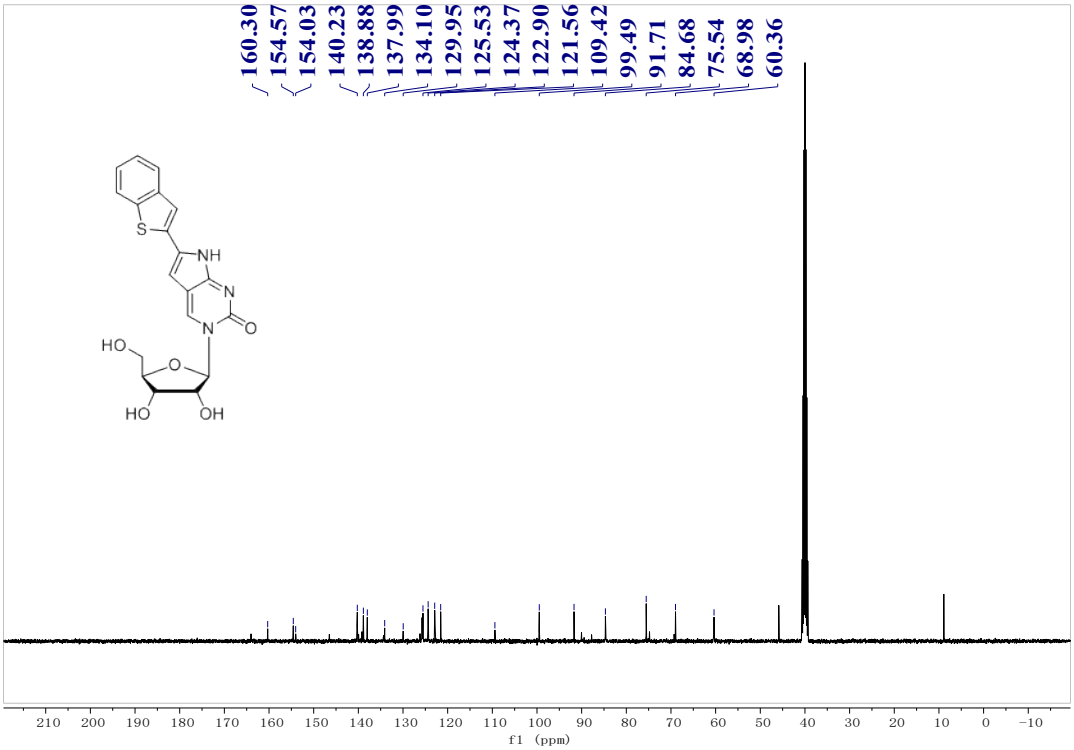

$^{13}$C NMR (101 MHz, DMSO): $\delta$ 161.6, 154.7, 150.0, 145.8, 138.2, 127.7, 126.5, 124.1, 122.1, 112.4, 111.6, 97.3, 89.2, 89.1, 85.2, 82.5, 74.5, 69.6, 60.5.

## $^{1}$H NMR Spectrum of Compound 4a.



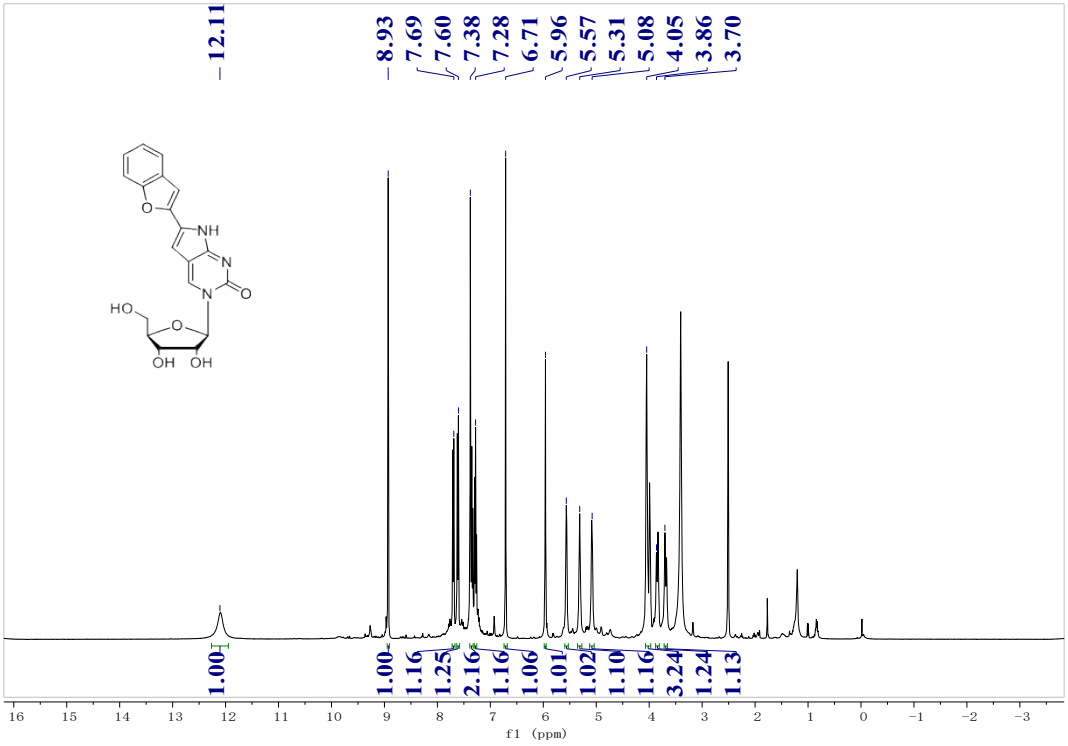

$^{1}$H NMR (400 MHz, DMSO): $\delta$ 12.10 (s, 1H), 8.88 (s, 1H), 7.98-7.95 (m, 1H), 7.96 (s, 1H), 7.85-7.82 (m, 1H), 7.39 (dd, $J$ = 7.4, 2.0 Hz, 2H), 6.60 (s, 1H), 5.95 (s, 1H), 5.54 (s, 1H), 5.32 (s, 1H), 5.10 (d, $J$ = 4.0 Hz, 1H), 4.06-3.99 (m, 3H), 3.82 (d, $J$ = 10.8 Hz, 1H), 3.70 (d, $J$ = 11.9 Hz, 1H).

## $^{13}$C NMR Spectrum of Compound 4a



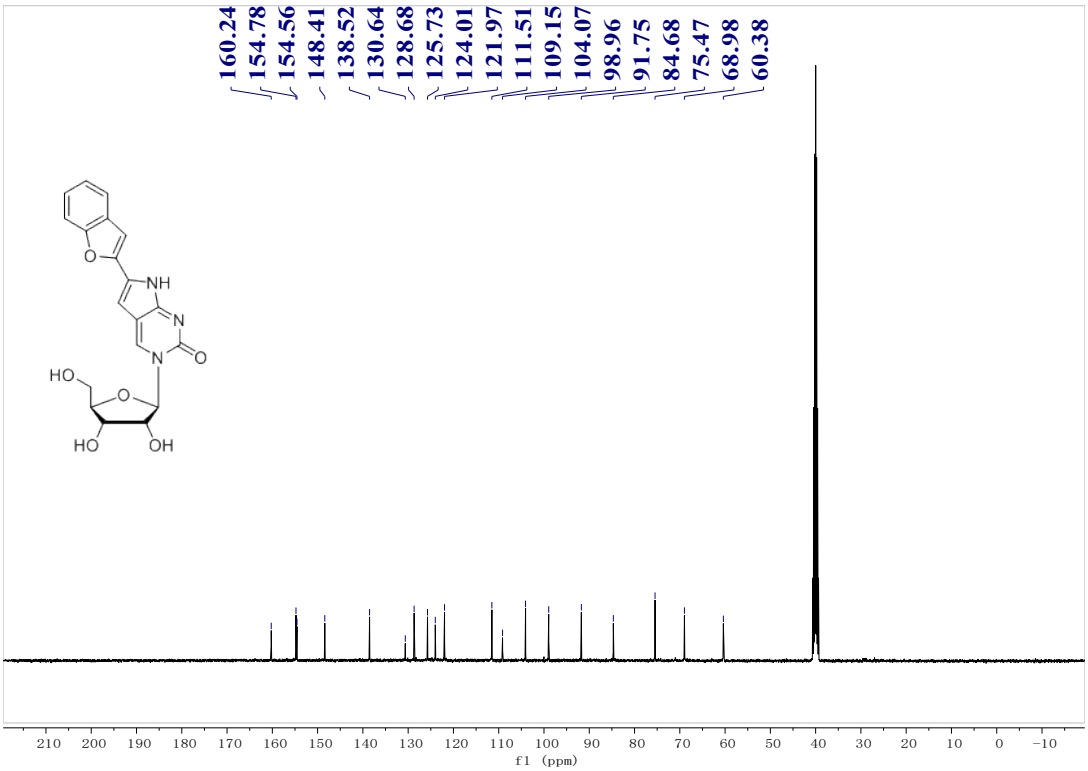

$^{13}$C NMR (101 MHz, DMSO): $\delta$ 160.3, 154.6, 154.0, 140.2, 138.9, 138.0, 134.1, 130.0, 125.5, 124.4, 122.9, 121.6, 109.4, 99.5, 91.7, 84.7, 75.5, 69.0, 60.4.

## $^{1}$H NMR Spectrum of Compound 4b



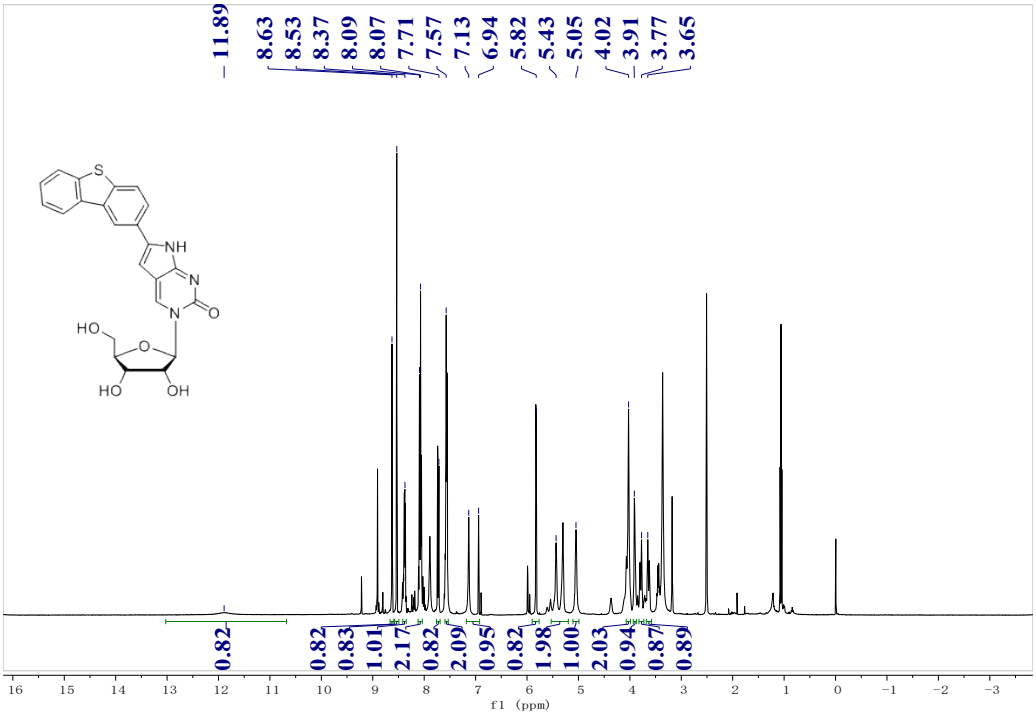

$^{1}$H NMR (400 MHz, DMSO): $\delta$ 12.11 (s, 1H), 8.93 (s, 1H), 7.69 (d, $J$ = 7.5 Hz, 1H), 7.60 (d, $J$ = 8.2 Hz, 1H), 7.39-7.32 (m, 2H), 7.28 (t, $J$ = 7.4 Hz, 1H), 6.71 (s, 1H), 5.96 (s, 1H), 5.57 (s, 1H), 5.31 (s, 1H), 5.08 (s, 1H), 4.05 (d, $J$ = 22.0 Hz, 3H), 3.86 (d, $J$ = 11.9 Hz, 1H), 3.70 (d, $J$ = 12.0 Hz, 1H).

## $^{13}$C NMR Spectrum of Compound 4b



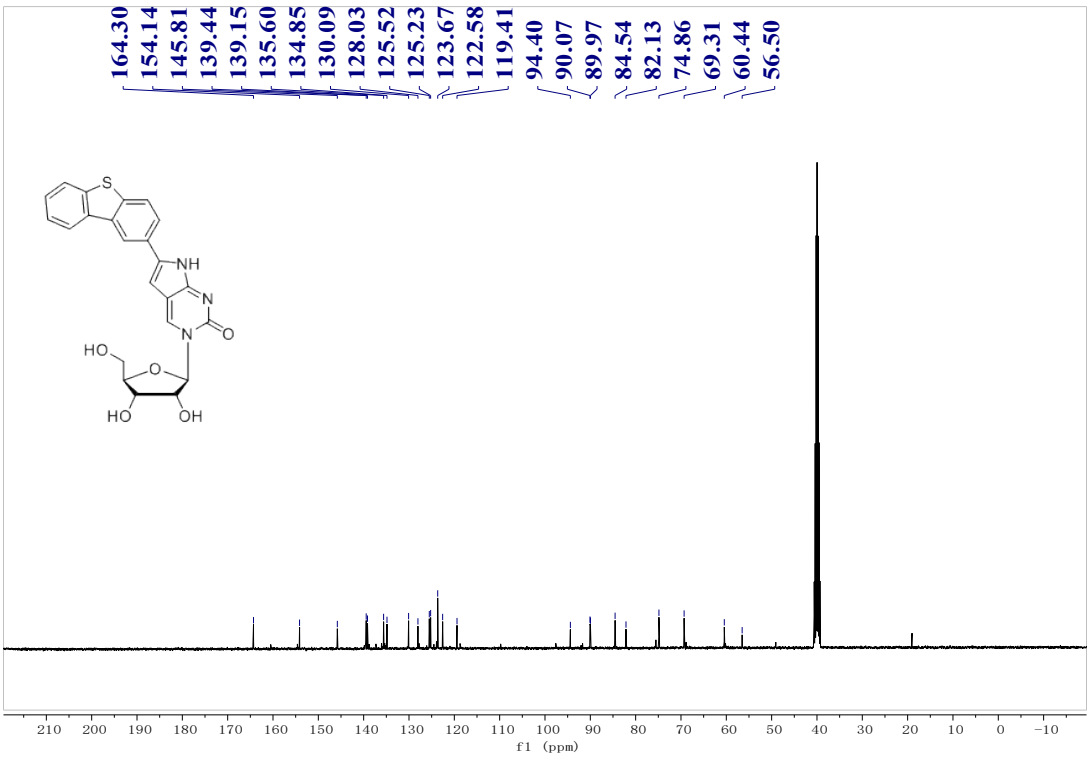

$^{13}$C NMR (101 MHz, DMSO): $\delta$ 160.2, 154.8, 154.6, 148.4, 138.5, 130.6, 128.7, 125.7, 124.0, 122.0, 111.5, 109.2, 104.1, 99.0, 91.8, 84.7, 75.5, 69.0, 60.4.

## $^{1}$H NMR Spectrum of Compound 4c



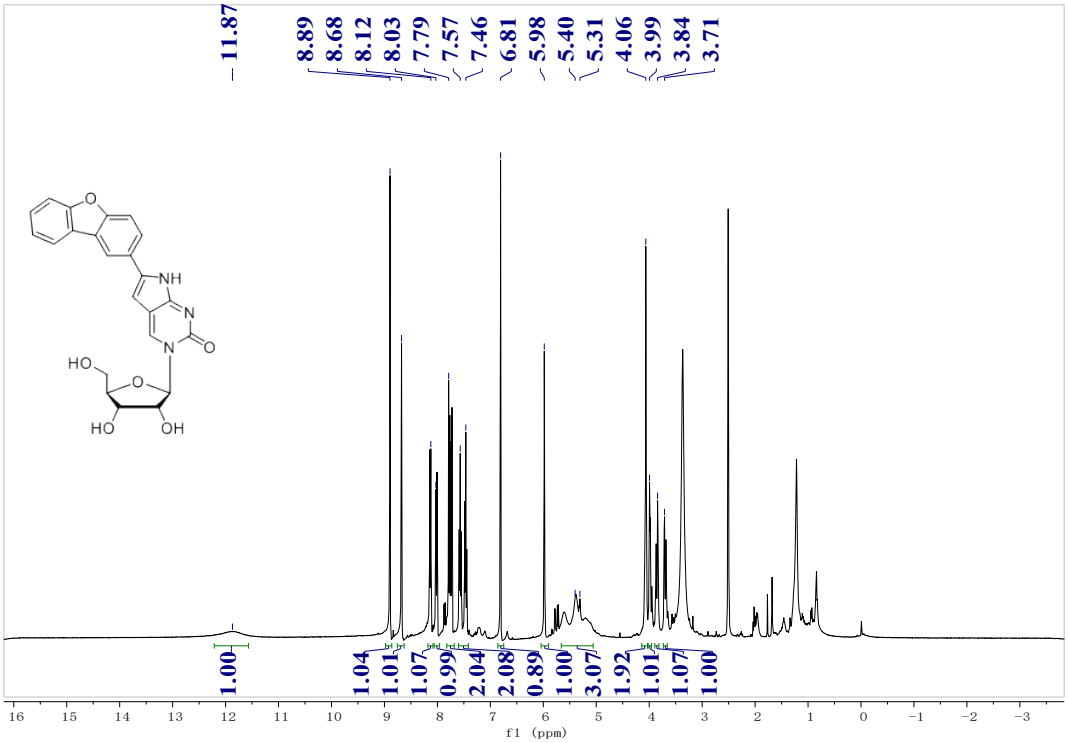

$^{1}$H NMR (400 MHz, DMSO): $\delta$ 11.89 (s, 1H), 8.63 (s, 1H), 8.53 (s, 1H), 8.37 (d, $J$ = 6.3, 2.8 Hz, 1H), 8.09-8.07 (t, $J$ = 7.8 Hz, 2H), 7.71 (d, $J$ = 8.3, 1.5 Hz, 1H), 7.57-7.13 (d, $J$ = 5.9, 3.3 Hz, 2H), 6.94 (d, $J$ = 76.8 Hz, 1H), 5.82 (d, $J$ = 3.2 Hz, 1H), 5.43 (d, $J$ = 52.9 Hz, 2H), 5.05 (s, 1H), 4.02 (s, 2H), 3.93-3.87 (m, 1H), 3.77 (d, $J$ = 11.9 Hz, 1H), 3.65 (d, $J$ = 12.0 Hz, 1H).

## $^{13}$C NMR Spectrum of Compound 4c



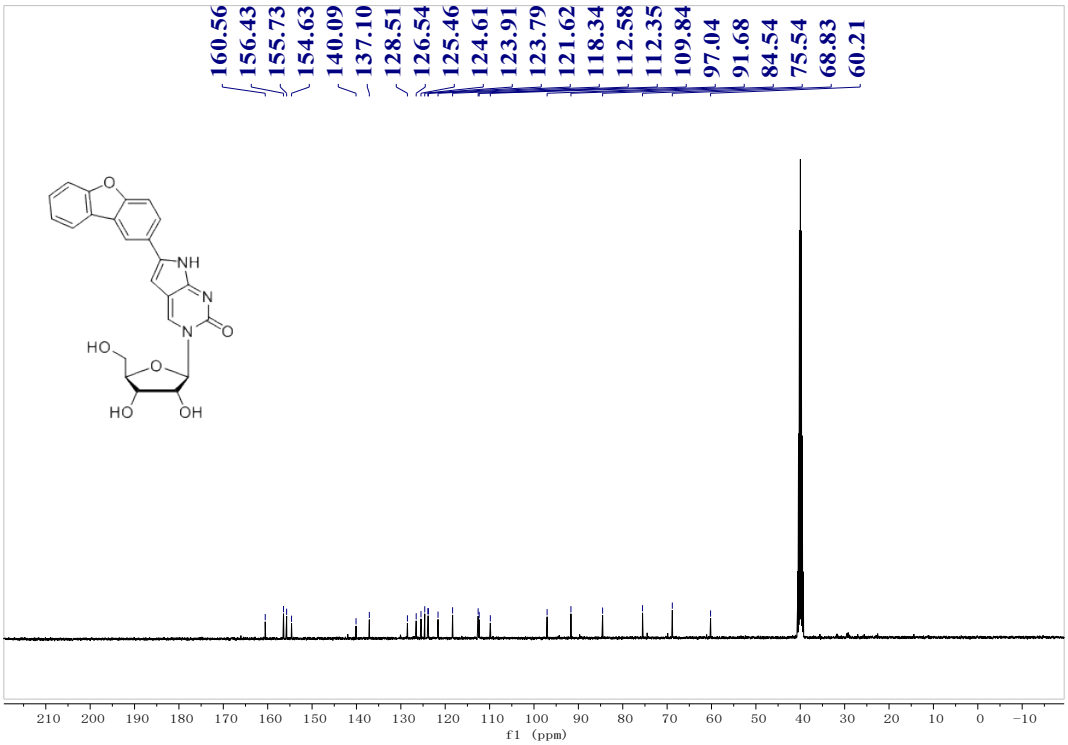

$^{13}$C NMR (101 MHz, DMSO): $\delta$ 164.3, 154.1, 145.8, 139.4, 139.2, 135.6, 134.9, 130.1, 128.0, 125.5, 125.2, 123.7, 122.6, 119.4, 94.4, 90.1, 90.0, 84.5, 82.1, 74.9, 69.3, 60.4, 56.5.

## $^{1}$H NMR Spectrum of Compound 4d



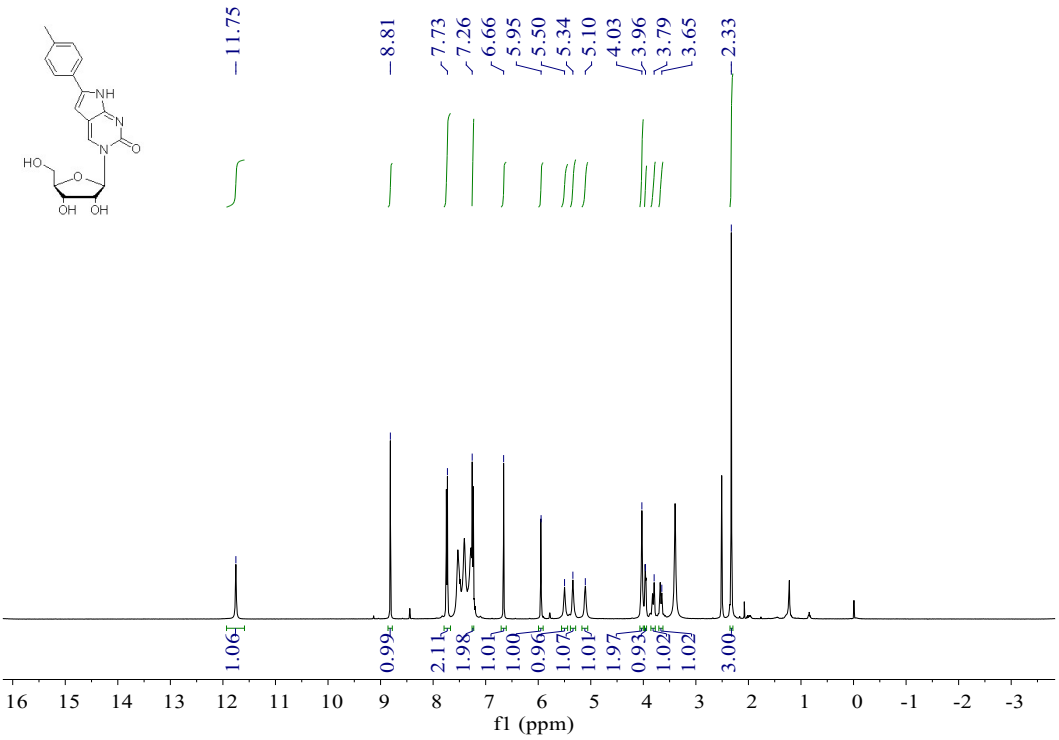

$^{1}$H NMR (400 MHz, DMSO): $\delta$ 11.87 (s, 1H), 8.89 (s, 1H), 8.68 (s, 1H), 8.12 (d, $J$ = 7.6 Hz, 1H), 8.03 (d, $J$ = 8.6 Hz, 1H), 7.79 (dd, $J$ = 16.9, 8.4 Hz, 2H), 7.57-7.46 (dt, $J$ = 42.1, 7.5 Hz, 2H), 6.81 (s, 1H), 5.98 (d, $J$ = 2.0 Hz, 1H), 5.66-5.06 (m, 3H), 4.06 (s, 2H), 4.02-3.96 (m, 1H), 3.84 (d, $J$ = 12.1 Hz, 1H), 3.71 (d, $J$ = 13.6 Hz, 1H).

## $^{13}$C NMR Spectrum of Compound 4d



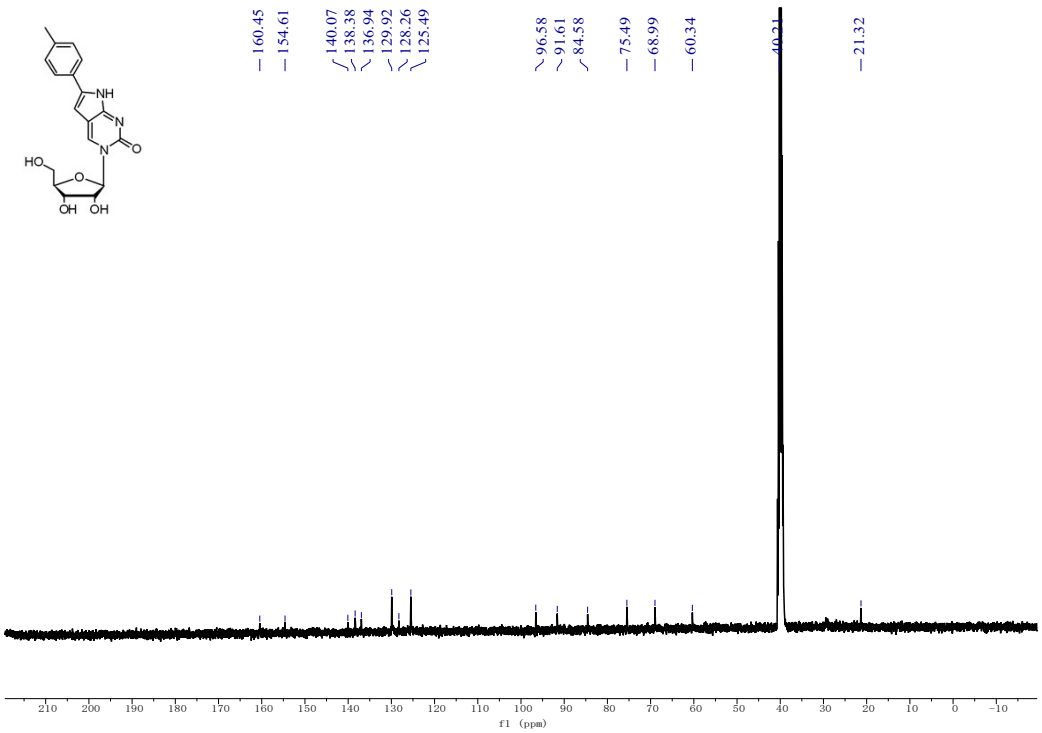

$^{13}$C NMR (101 MHz, DMSO): $\delta$ 160.6, 156.4, 155.7, 154.6, 140.1, 137.1, 128.5, 126.5, 125.5, 124.6, 123.9, 123.8, 121.6, 118.3, 112.6, 112.4, 109.8, 97.0, 91.7, 84.5, 75.5, 68.8, 60.2.

## $^{1}$H NMR Spectrum of Compound 4e



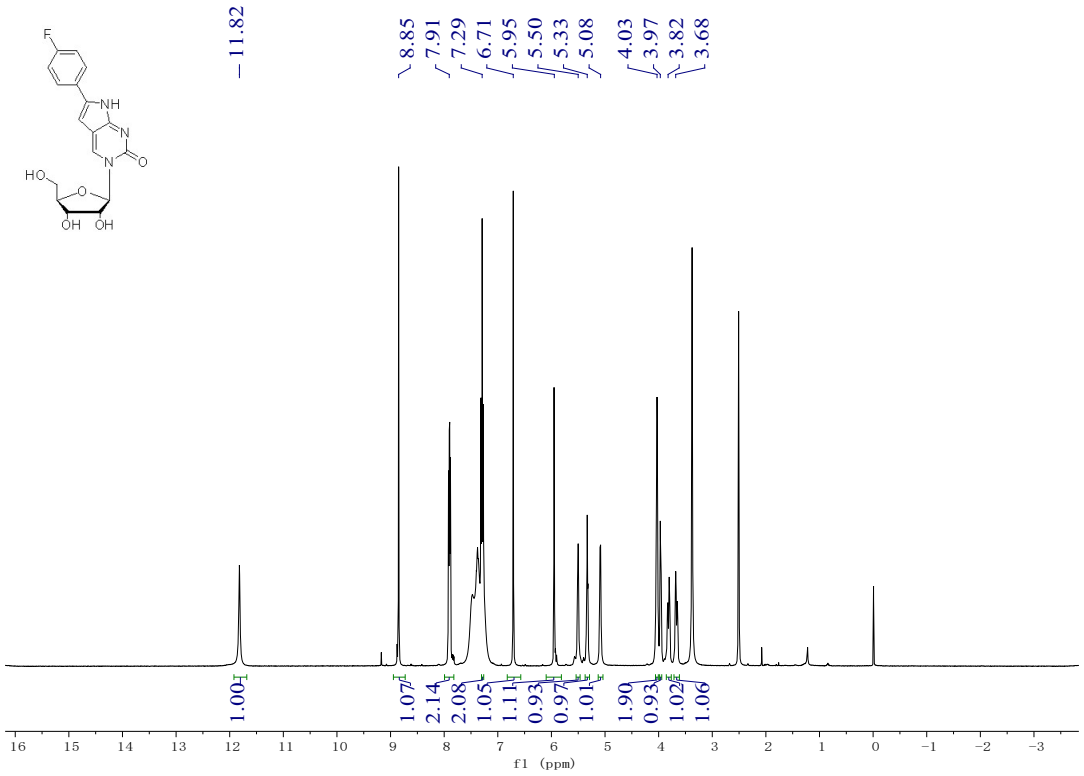

$^{1}$H NMR (400 MHz, DMSO-*d6*) $\delta$ 11.75 (s, 1H), 8.81 (s, 1H), 7.73 (d, $J$ = 8.1 Hz, 2H), 7.26 (d, $J$ = 8.1 Hz, 2H), 6.66 (s, 1H), 5.95 (s, 1H), 5.50 (s, 1H), 5.34 (s, 1H), 5.10 (s, 1H), 4.03 (s, 2H), 3.98-3.94 (m, 1H), 3.79 (s, 1H), 3.65 (s, 1H), 2.33 (s, 3H).

## $^{13}$C NMR Spectrum of Compound 4e



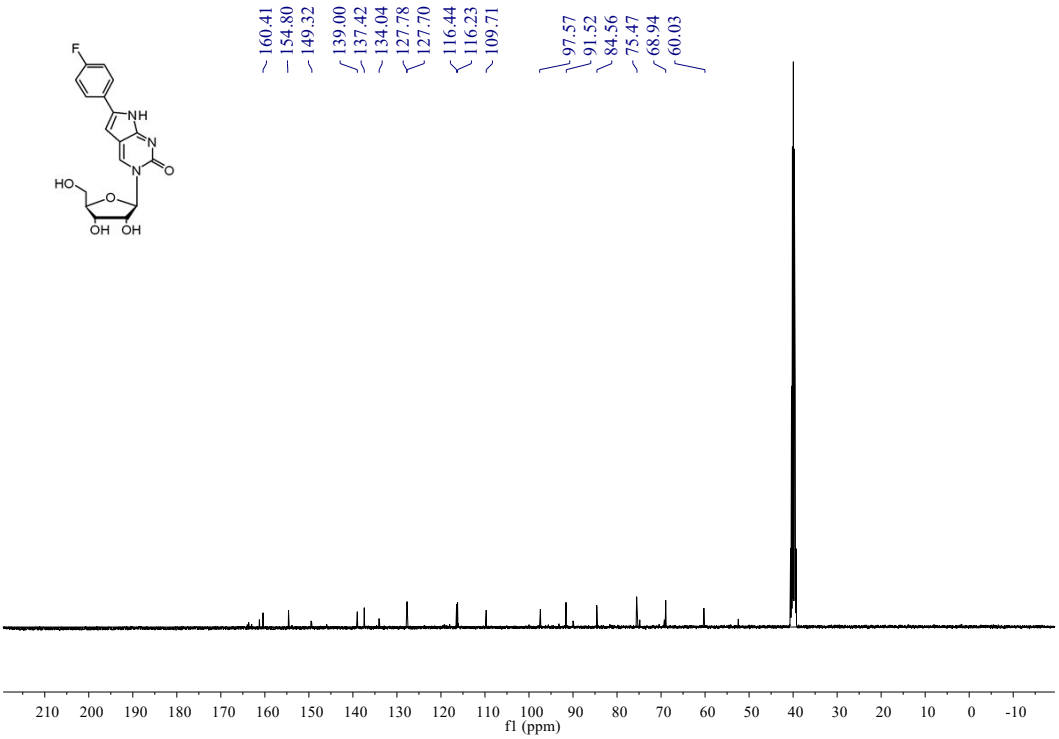

$^{13}$C NMR (101 MHz, DMSO-*d6*) $\delta$ 160.5, 154.6, 140.1, 138.4, 136.9, 129.9, 128.3, 125.5, 96.6, 91.6, 84.6, 75.5, 69.0, 60.3, 21.3.

## $^{1}$H NMR Spectrum of Compound 4f



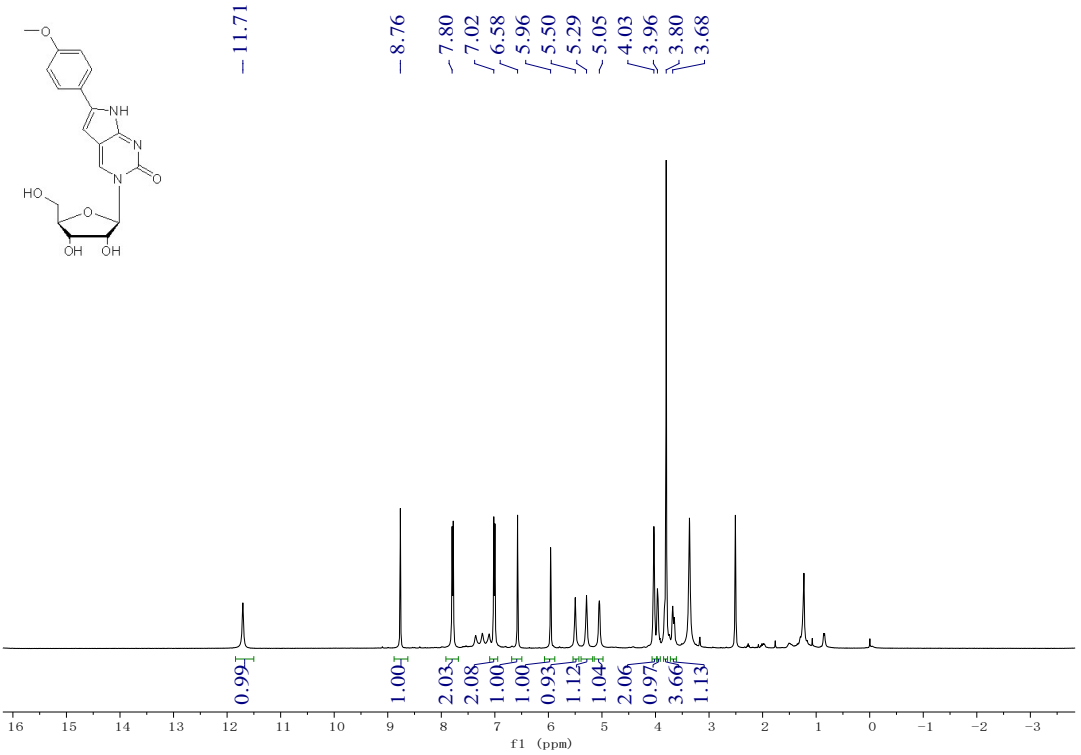

$^{1}$H NMR (400 MHz, DMSO-*d6*) $\delta$ 11.82 (s, 1H), 8.85 (s, 1H), 8.01-7.82 (m, 2H), 7.32-7.27 (m, 2H), 6.71 (s, 1H), 5.95 (s, 1H), 5.50 (s, 1H), 5.33 (s, 1H), 5.08 (s, 1H), 4.03-3.97 (d, $J$ = 25.6 Hz, 3H), 3.82 (d, $J$ = 10.6 Hz, 1H), 3.71-3.56 (m, 1H).

## $^{13}$C NMR Spectrum of Compound 4f



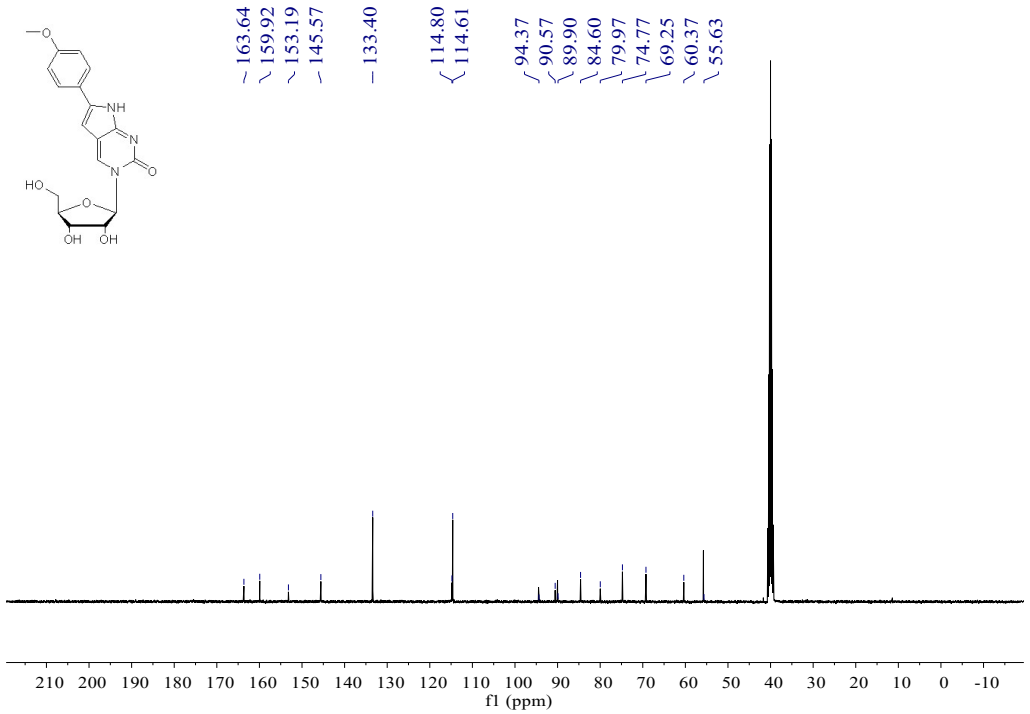

$^{13}$C NMR (101 MHz, DMSO-*d6*) $\delta$ 160.4, 154.8, 149.3, 139.0, 137.4, 134.0, 127.8, 116.4, 116.2, 109.7, 97.6, 91.5, 84.6, 75.5, 68.945, 60.0.

## $^{1}$H NMR Spectrum of Compound 4g



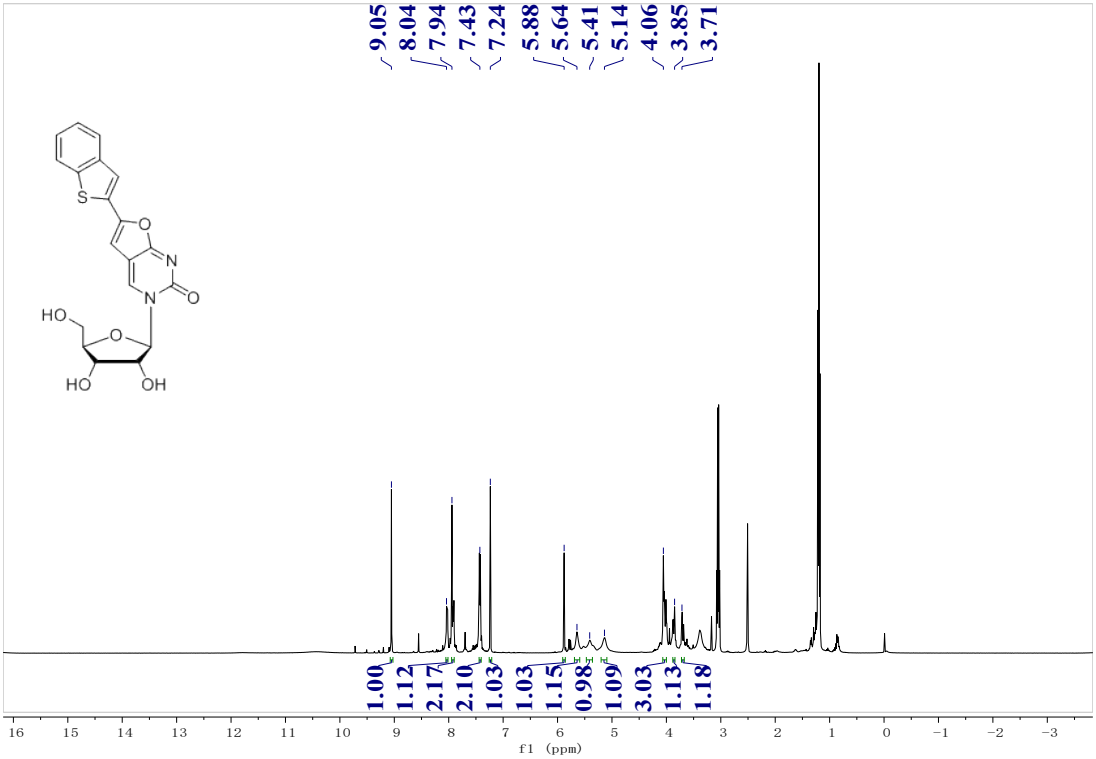

$^{1}$H NMR (400 MHz, DMSO-*d6*) $\delta$ 11.71 (s, 1H), 8.76 (s, 1H), 7.80 (d, $J$ = 8.6 Hz, 2H), 7.02 (d, $J$ = 8.6 Hz, 2H), 6.58 (s, 1H), 5.96 (s, 1H), 5.50 (s, 1H), 5.29 (s, 1H), 5.05 (s, 1H), 4.03 (s, 2H), 3.96 (s, 1H), 3.80 (s, 3H), 3.72-3.61 (m, 1H).

## $^{13}$C NMR Spectrum of Compound 4g



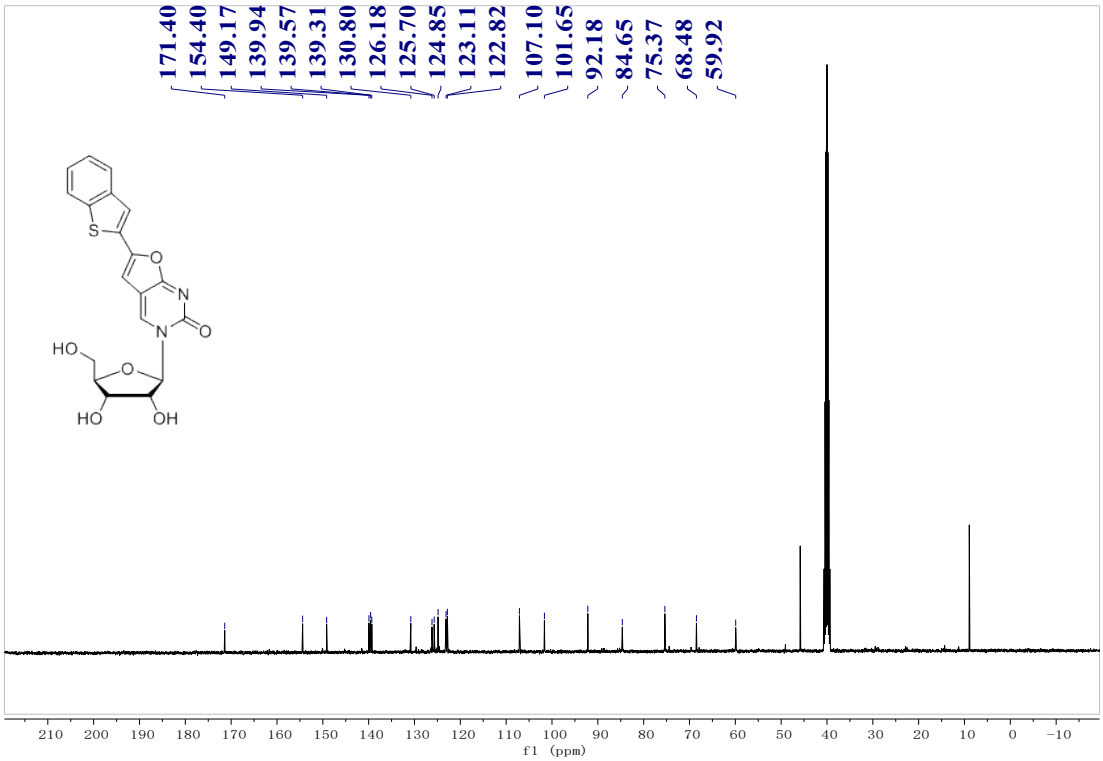

$^{13}$C NMR (101 MHz, DMSO-*d6*) $\delta$ 163.6, 159.9, 153.2, 145.6, 133.4, 114.8, 114.6, 94.4, 90.6, 89.9, 84.6, 80.0, 74.8, 69.3, 60.4, 55.6.

## $^{1}$H NMR Spectrum of Compound 4h



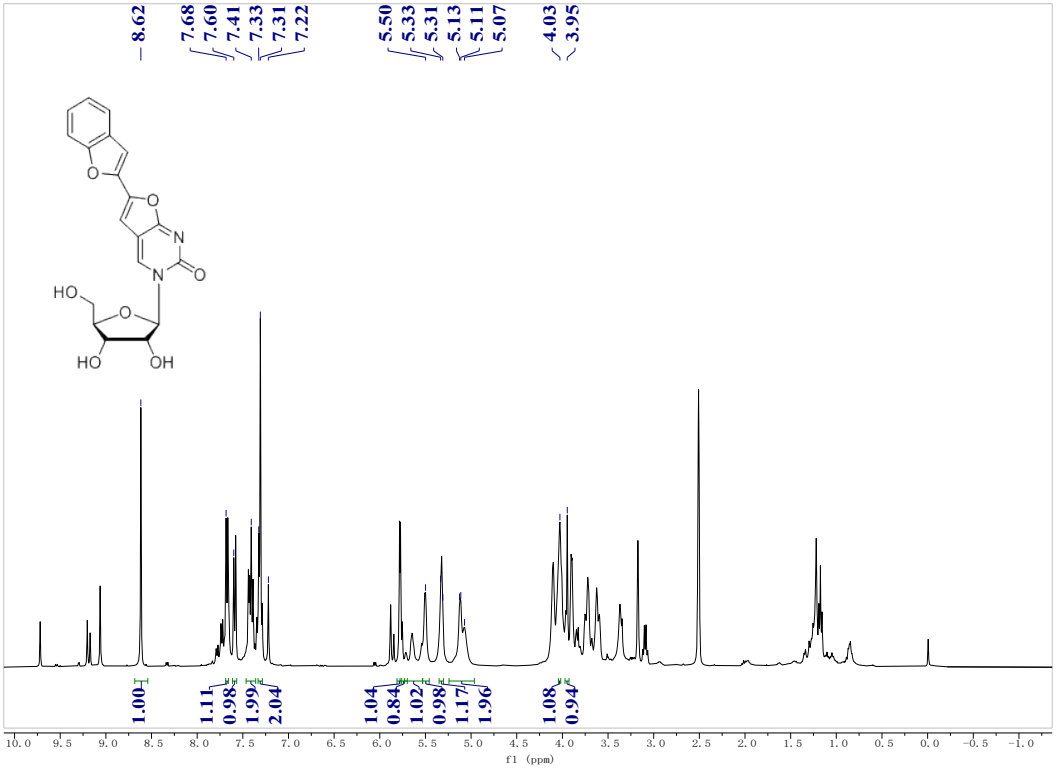

$^{1}$H NMR (400 MHz, DMSO): $\delta$ 9.05 (s, 1H), 8.05-8.01 (m, 1H), 7.95 -7.90 (m, 2H), 7.44-7.40 (m, 2H), 7.24 (s, 1H), 5.88 (s, 1H), 5.64 (s, 1H), 5.41 (s, 1H), 5.14 (s, 1H), 4.07-4.00 (m, 3H), 3.85 (d, $J$ = 12.2 Hz, 1H), 3.71 (d, $J$ = 12.0 Hz, 1H).

## $^{13}$C NMR Spectrum of Compound 4h



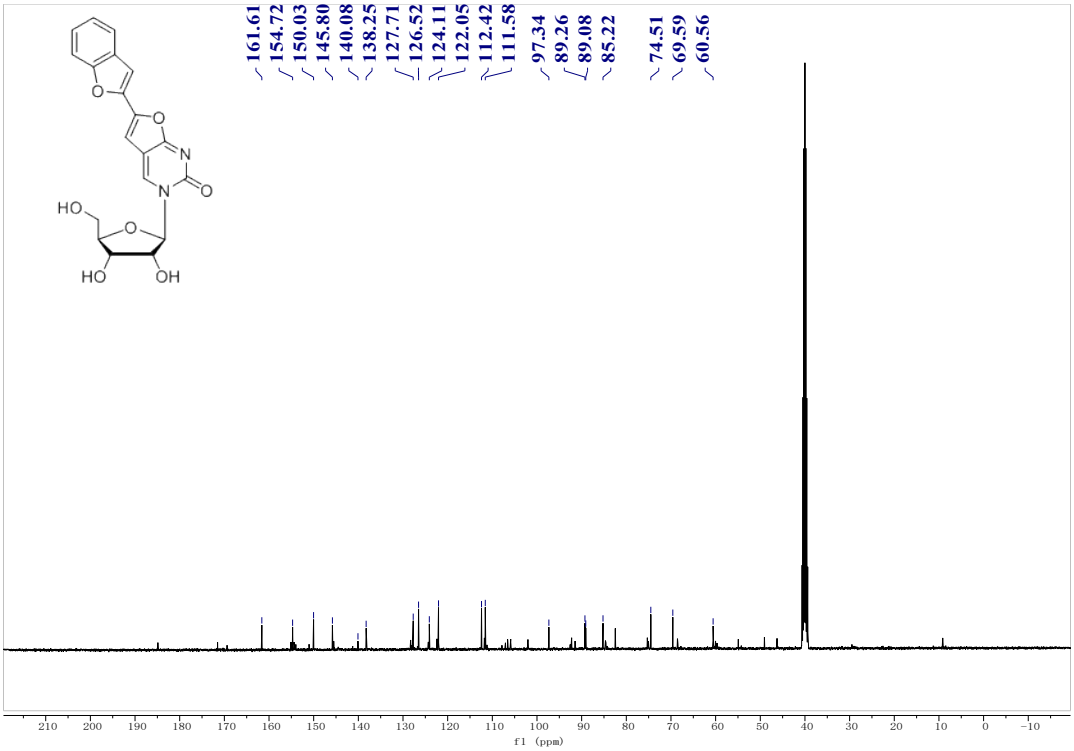

$^{13}$C NMR (101 MHz, DMSO): $\delta$ 171.4, 154.4, 149.2, 139.9, 139.6, 139.3, 130.8, 126.2, 125.7, 124.9, 123.1, 122.8, 107.1, 101.7, 92.2, 84.7, 75.4, 68.5, 59.9.

## $^{1}$H NMR Spectrum of Compound 4i




$^{1}$H NMR (400 MHz, DMSO): $\delta$ 8.62 (s, 1H), 7.68 (d, $J$ = 7.5 Hz, 1H), 7.60 (d, $J$ = 8.2 Hz, 1H), 7.41 (dd, $J$ = 13.8, 6.5 Hz, 2H), 7.33-7.22 (m, 2H), 5.50 (s, 1H), 5.33 (s, 1H), 5.31 (s, 1H), 5.13 (d, $J$ = 19.6 Hz, 1H), 5.11 (s, 1H), 5.07(m,2H), 4.03 (s, 1H), 3.95 (s, 1H).

## $^{13}$C NMR Spectrum of Compound 4i




$^{13}$C NMR (101 MHz, DMSO): $\delta$ 161.6, 154.7, 150.0, 145.8, 140.1, 138.3, 127.7, 126.5, 124.1, 122.1, 112.4, 111.6, 97.3, 89.3, 89.1, 85.2, 74.5, 69.6, 60.6.

## 6. MS spectra for products

**MS of C**

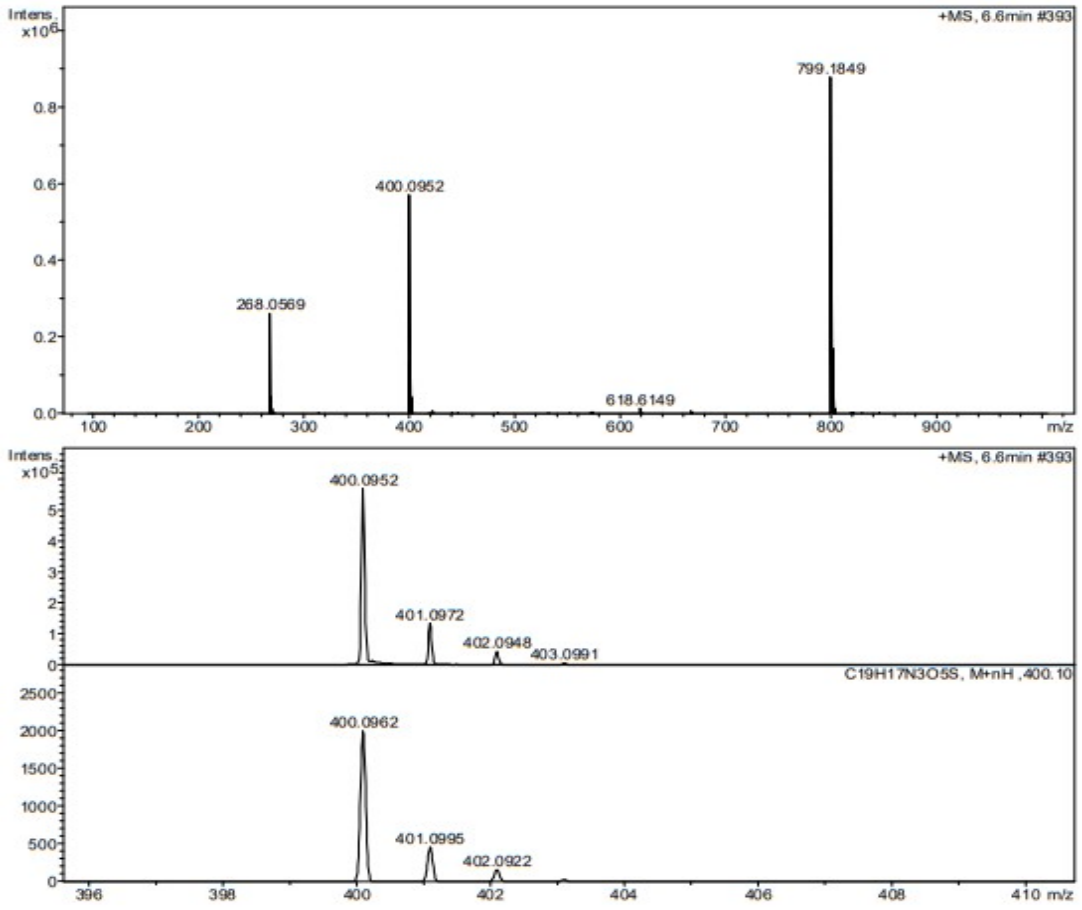
Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\2019MS\HJQ\0320\237_BA7_01_6339.d | Acquisition Date | 3/20/2019 11:00:08 AM |
| Method | tune_200-800_hcoona-pos-10min.m | Operator | gftang |
| Sample Name | 237 | Instrument / Ser# | micrOTOF II 10257 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 1.0 Bar |
| Focus | Not active | | | Set Dry Heater | 250 °C |
| Scan Begin | 100 m/z | Set Capillary | 4000 V | Set Dry Gas | 4.0 l/min |
| Scan End | 1000 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |

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**MS of**

# Display Report

**Analysis Info**

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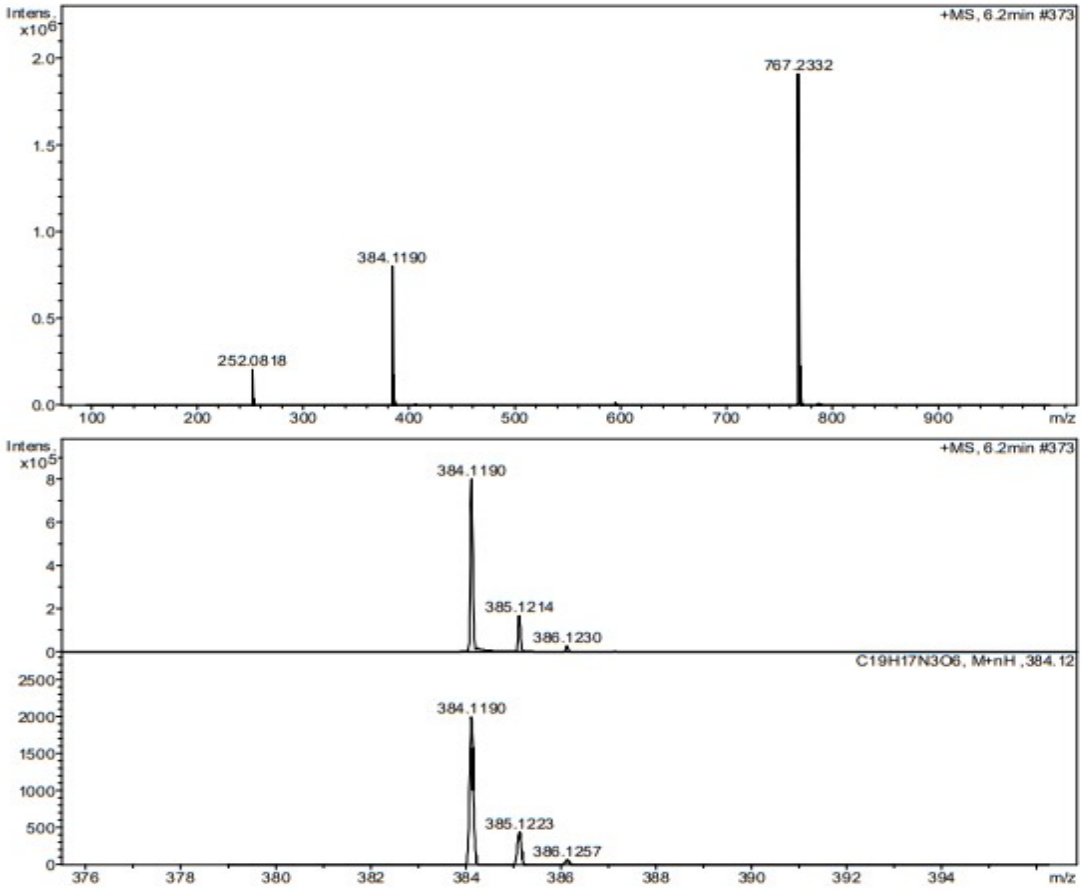
| Analysis Name | D:\Data\2019MS\HJQ\0320\234_BA6_01_6338.d | Acquisition Date | 3/20/2019 10:43:53 AM |
| Method | tune_200-800_hcoona-pos-10min.m | Operator | gftang |
| Sample Name | 234 | Instrument / Ser# | micrOTOF II 10257 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 1.0 Bar |
| Focus | Not active | | | Set Dry Heater | 250 °C |
| Scan Begin | 100 m/z | Set Capillary | 4000 V | Set Dry Gas | 4.0 l/min |
| Scan End | 1000 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |



**MS of Compou**

# Display Report

**Analysis Info**

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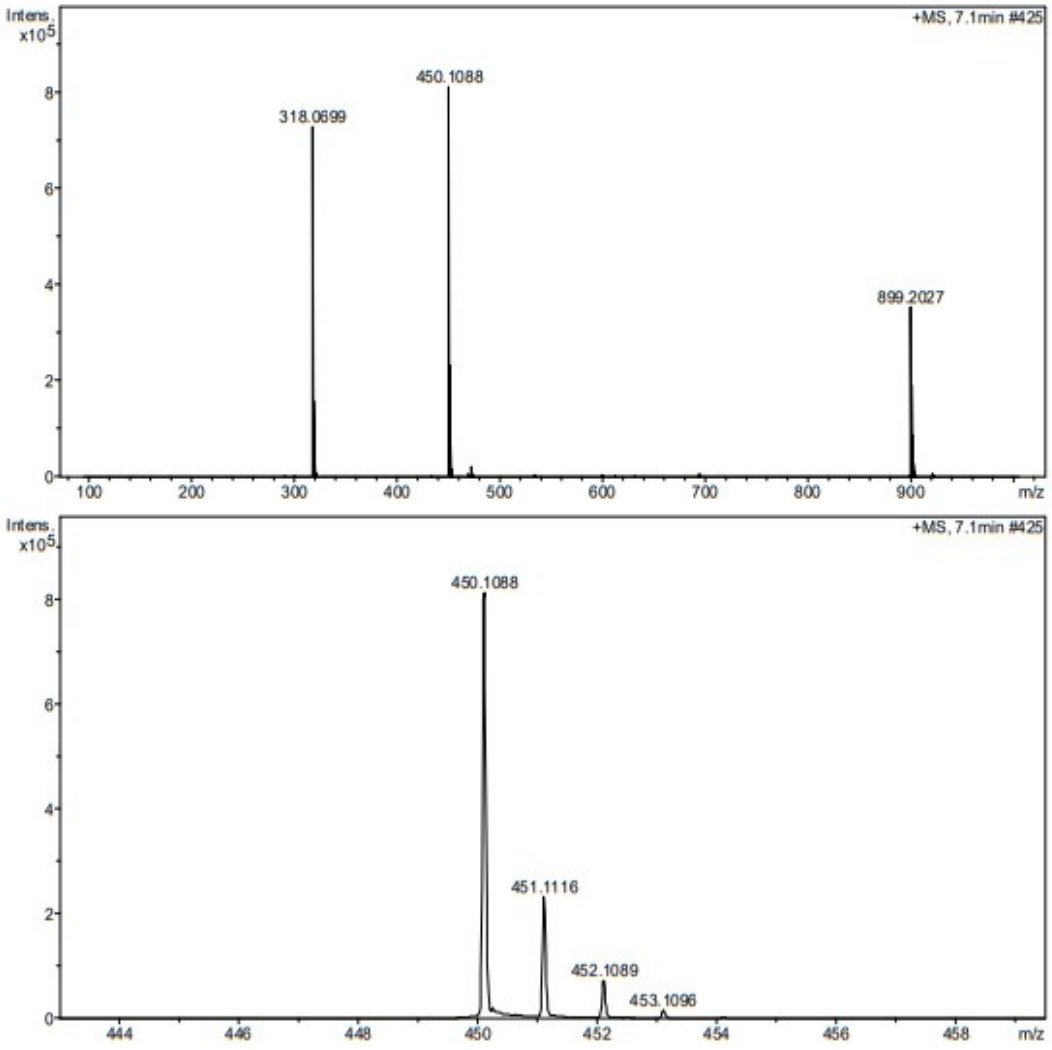
|---|---|---|---|
| Analysis Name | D:\Data\2019MS\HJQ\0320\296_BB2_01_6342.d | Acquisition Date | 3/20/2019 11:48:54 AM |
| Method | tune_200-800_hcoona-pos-10min.m | Operator | gftang |
| Sample Name | 296 | Instrument / Ser# | micrOTOF II 10257 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 1.0 Bar |
| Focus | Not active | | | Set Dry Heater | 250 °C |
| Scan Begin | 100 m/z | Set Capillary | 4000 V | Set Dry Gas | 4.0 l/min |
| Scan End | 1000 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |

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**MS of Compo**

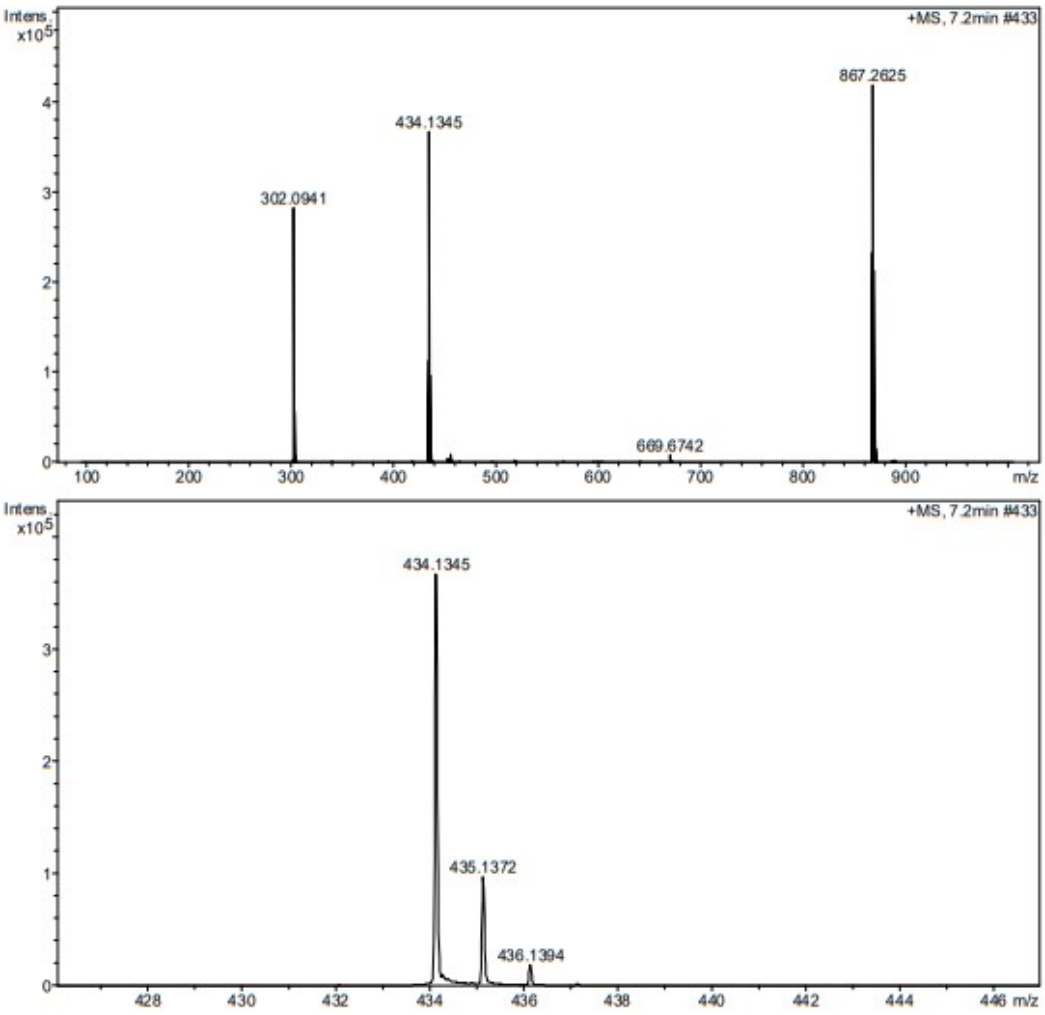
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\2019MS\HJQ\0320\297_BB3_01_6343.d | Acquisition Date | 3/20/2019 12:05:10 PM |
| Method | tune_200-800_hcoona-pos-10min.m | Operator | gftang |
| Sample Name | 297 | Instrument / Ser# | micrOTOF II 10257 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 1.0 Bar |
| Focus | Not active | | | Set Dry Heater | 250 °C |
| Scan Begin | 100 m/z | Set Capillary | 4000 V | Set Dry Gas | 4.0 l/min |
| Scan End | 1000 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |

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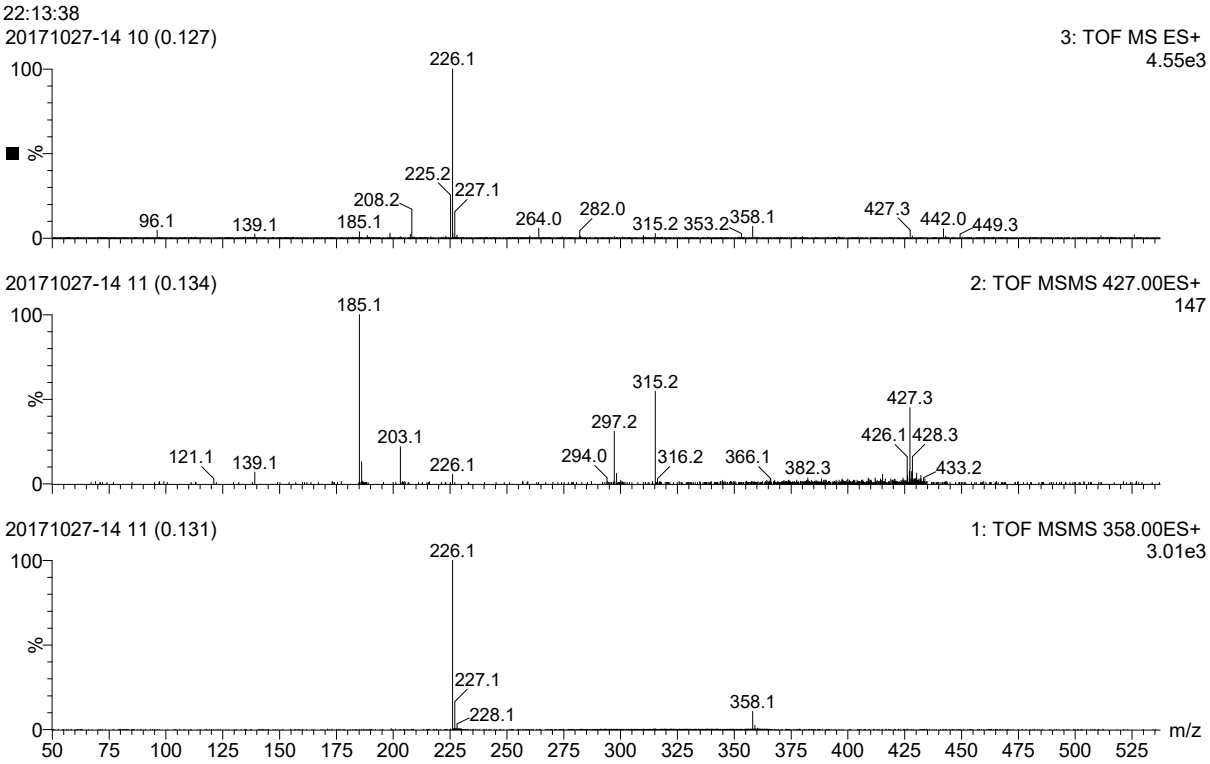
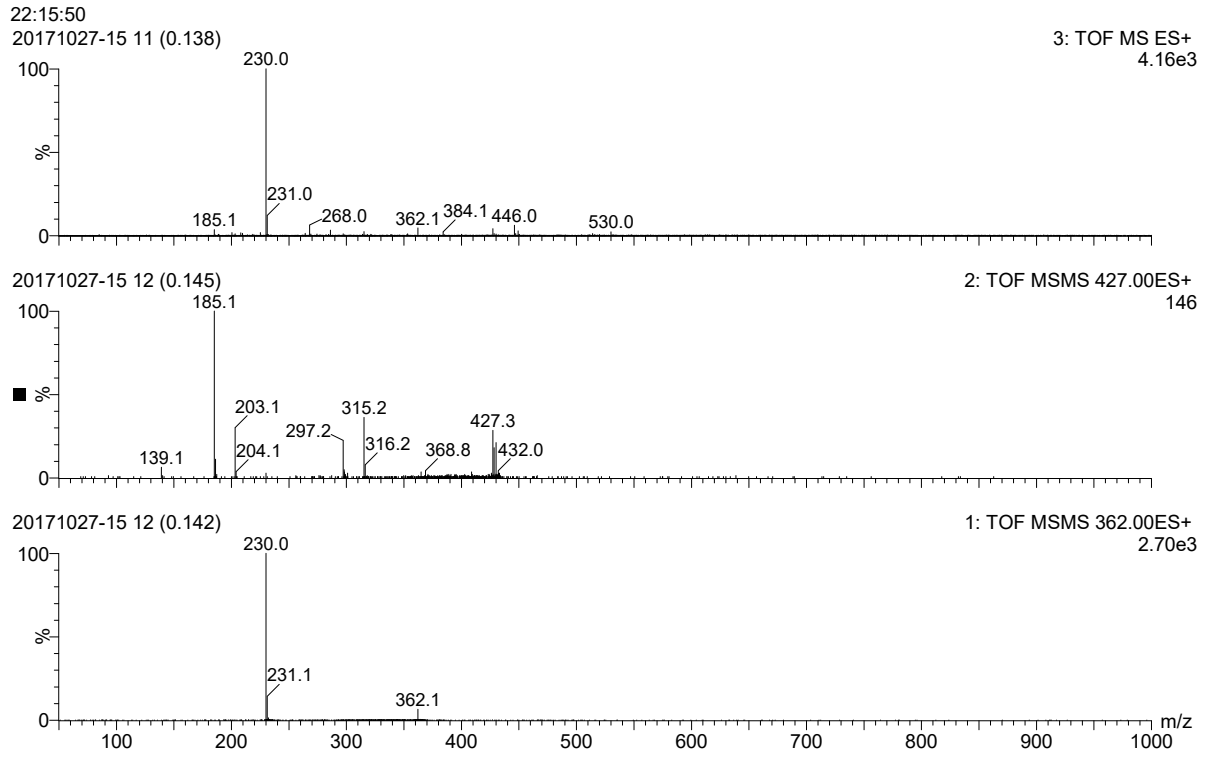
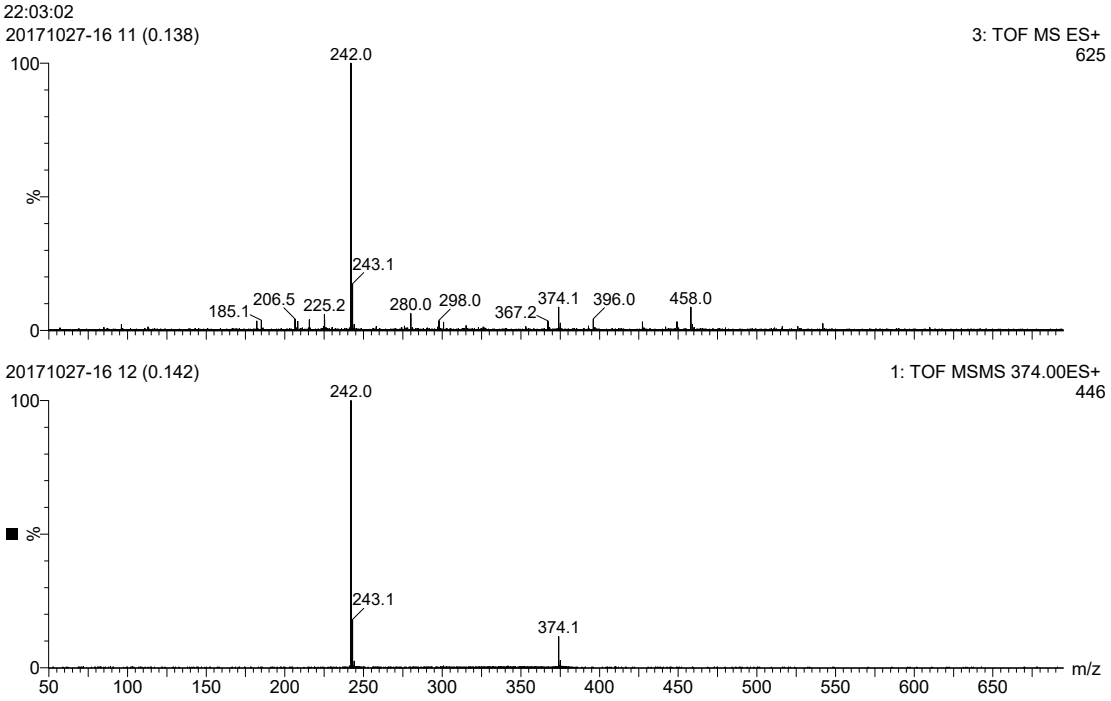
## MS of Compound 4e




## MS of Compound 4f



## MS of Compound 4g



**MS of Compou**

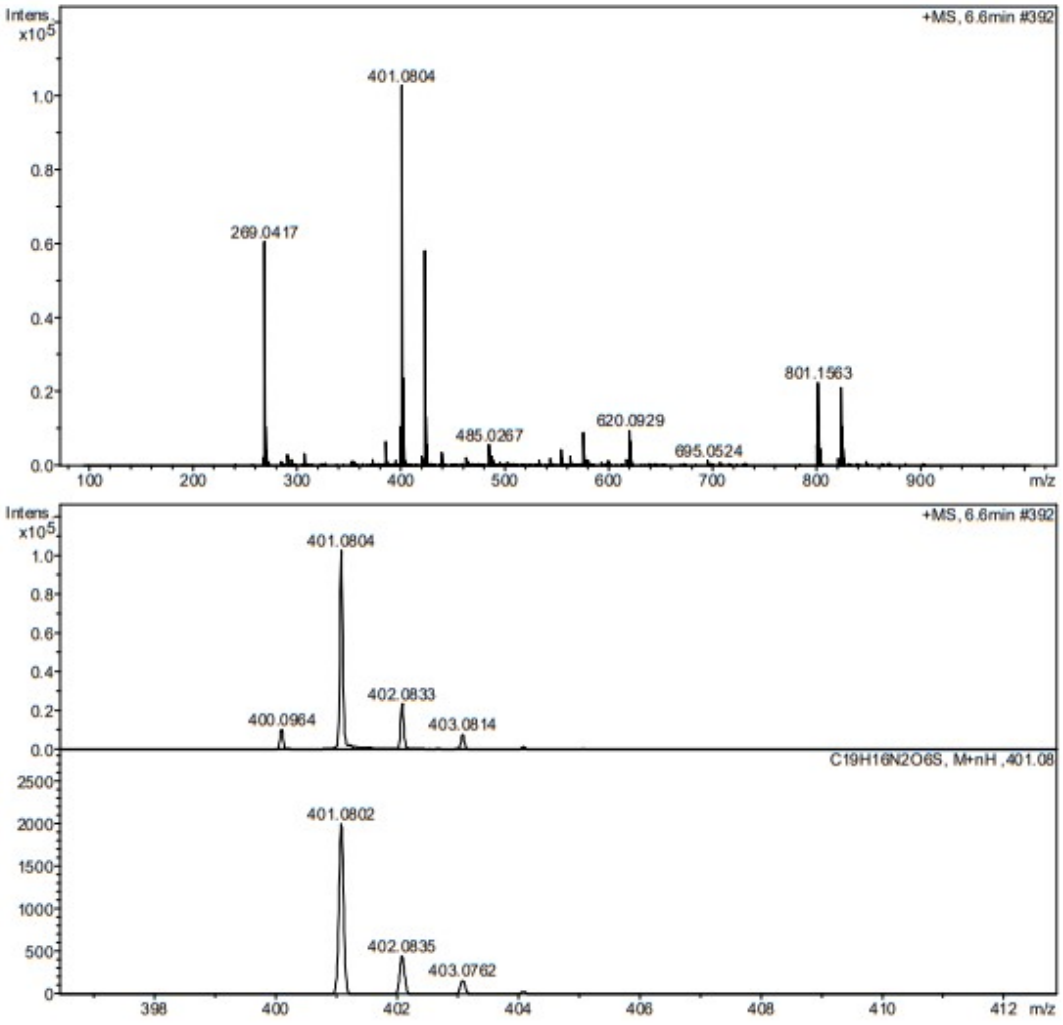
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\2019MS\HJQ\0320\248_BA8_01_6340.d | Acquisition Date | 3/20/2019 11:16:23 AM |
| Method | tune_200-800_hcoona-pos-10min.m | Operator | gftang |
| Sample Name | 248 | Instrument / Ser# | micrOTOF II 10257 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 1.0 Bar |
| Focus | Not active | | | Set Dry Heater | 250 °C |
| Scan Begin | 100 m/z | Set Capillary | 4000 V | Set Dry Gas | 4.0 l/min |
| Scan End | 1000 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |



**MS of Compou**

# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\2019MS\HJQ\0320\250_BB1_01_6341.d | Acquisition Date | 3/20/2019 11:32:39 AM |
| Method | tune_200-800_hcoona-pos-10min.m | Operator | gftang |
| Sample Name | 250 | Instrument / Ser# | micrOTOF II 10257 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 1.0 Bar |
| Focus | Not active | | | Set Dry Heater | 250 °C |
| Scan Begin | 100 m/z | Set Capillary | 4000 V | Set Dry Gas | 4.0 l/min |
| Scan End | 1000 m/z | Set End Plate Offset | -500 V | Set Divert Valve | Waste |