

Pyruvic Acid or DBU/O₂ Guiding Organophotoredox-Catalyzed Direct C-H Alkylation/ α -Aminoalkylation of 1,2,4-Triazine-3,5(2*H*, 4*H*)-diones with Amines

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Supporting Information

Table of Contents

I. General methods and materials.....	2
II. Synthesis of substrates.....	2
III. General procedure.....	2
IV. Optimization of reaction conditions.....	3
V. Unsuitable (hetero)aromatic cycles and amines.....	4
VI. Procedure for emission quenching experiments.....	4
VII. Mechanistic Experiments.....	5
VIII. Scale-up experiment.....	7
IX. Characterization data of 3a-4aa	8
X. NMR charts of 3a-4u	21
XI. Computational details.....	72
XII. References.....	92

I. General methods and materials

All manipulations were performed under an air atmosphere unless otherwise stated. ^1H and ^{13}C NMR spectra were recorded on a Bruker AC-P 400 spectrometer (400 MHz for ^1H , 100 MHz for ^{13}C) in CDCl_3 . Chemical shifts (ppm) were recorded with tetramethylsilane (TMS) as the internal reference standard. Multiplicities are given as: s (singlet), d (doublet), t (triplet), dd (doublet of doublets), q (quartet) or m (multiplet). Copies of their ^1H NMR and ^{13}C NMR spectra are provided in the Supporting Information. High resolution mass spectra (HRMS) were recorded on quadrupole time-of-flight mass spectrometer (Q-TOF-MS) using electrospray ionization (ESI) as an ionization method. Emission intensities were recorded using an FS5 Spectrofluorometer. Solvents were dried and purified according to the procedure from "Purification of Laboratory Chemicals book". The crude products were purified by flash column chromatography on silica gel and the reported yields are the actual isolated yields of pure products. Unless stated otherwise, commercial reagents were used without further purification. All reagents were weighed and handled in air at room temperature.

II. Synthesis of substrates

General Procedure for the Preparation of various 1,2,4-Triazine-3,5(2*H*,4*H*)-diones

The substrates of various 1,2,4-triazine-3,5(2*H*,4*H*)-diones were synthesized according to procedures described in the previous literature studies.^{1,2}

III. General procedure

Procedure for the Synthesis of **3a**

To a solution of 2,4-dibenzyl-1,2,4-triazine-3,5(2*H*, 4*H*)-dione **1a** (0.3 mmol) and 4CzIPN (5 mol%) in DMC (3 mL) were placed in a flame-dried Schlenk-tube equipped with a magnetic stir bar, followed by addition of pyruvic acid (1.5 equiv.) and diethylamine **2a** (0.6 mmol) *via* syringe. The reaction was stirred at room temperature and irradiated with a 20 W blue light-emitting diode (LED) lamp for 12 h. The progress of the reaction was monitored by TLC. After completion, the reaction mixture was removed under reduced pressure. The crude residue thus obtained was purified by column chromatography over silica gel using petroleum ether and ethyl acetate (25:1) as an eluent to afford the 2,4-dibenzyl-6-ethyl-1,2,4-triazine-3,5(2*H*, 4*H*)-dione **3a** in 91% yield.

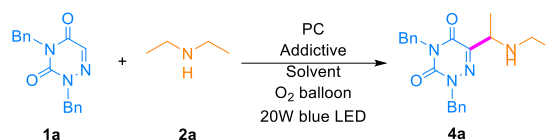
Procedure for the Synthesis of **4a**

To a solution of 2,4-dibenzyl-1,2,4-triazine-3,5(2*H*, 4*H*)-dione **1a** (0.3 mmol) and 4CzIPN (5 mol%) in DCM (3 mL) were placed in a flame-dried Schlenk-tube equipped with a magnetic stir bar, followed by addition of DBU (2.0 equiv.) and diethylamine **2a** (0.9 mmol) *via* syringe. The reaction was stirred at room temperature under O_2 atmosphere and irradiated with a 20 W blue light-emitting diode (LED) lamp for 6 h. The progress of the reaction was monitored by TLC. After completion, the reaction

mixture was removed under reduced pressure. The crude residue thus obtained was purified by column chromatography over silica gel using petroleum ether and ethyl acetate (1:1) as an eluent to afford the 2,4-dibenzyl-6-(1-(ethylamino)ethyl)-1,2,4-triazine-3,5(2*H*, 4*H*)-dione **4a** in 79% yield.

IV. Optimization of reaction conditions

Table S1 Optimization of reaction conditions for the preparation of **4a**



Entry	Photocatalyst (mol%)	Base (equiv.)	Solvent (mL)	4a Yield (%) ^[a]
1 ^[b]	4CzIPN (5.0)	DBU (2.0)	DMC (3.0)	27
2 ^[b]	4CzIPN (5.0)	DBU (2.0)	DCM (3.0)	52
3 ^[b]	4CzIPN (5.0)	DBU (2.0)	DCE (3.0)	50
4 ^[b]	4CzIPN (5.0)	DBU (2.0)	H2O (3.0)	0
5 ^[b]	4CzIPN (5.0)	DBU (2.0)	EtOH (3.0)	0
6 ^[c]	4CzIPN (5.0)	DBU (2.0)	DCM (3.0)	63
7	4CzIPN (5.0)	DBU (2.0)	DCM (3.0)	79
8	EoSinY (5.0)	DBU (2.0)	DCM (3.0)	0
9	(Mes-Acr-Me) ⁺ ClO ₄ ⁻ (5.0)	DBU (2.0)	DCM (3.0)	17
10	RoseBengal (5.0)	DBU (2.0)	DCM (3.0)	0
11	4CzPN (5.0)	DBU (2.0)	DCM (3.0)	53
12	5CzPN (5.0)	DBU (2.0)	DCM (3.0)	27
13	4CzIPN (5.0)	TMG (2.0)	DCM (3.0)	0
14	4CzIPN (5.0)	DBN (2.0)	DCM (3.0)	35
15	4CzIPN (5.0)	Pyridine (2.0)	DCM (3.0)	0
16	4CzIPN (5.0)	K ₃ PO ₄ (2.0)	DCM (3.0)	20
17	4CzIPN (5.0)	K ₂ CO ₃ (2.0)	DCM (3.0)	0
18	4CzIPN (3.0)	DBU (2.0)	DCM (3.0)	58
19	4CzIPN (7.0)	DBU (2.0)	DCM (3.0)	77
20	4CzIPN (5.0)	DBU (1.5)	DCM (3.0)	60
21	4CzIPN (5.0)	DBU (2.5)	DCM (3.0)	79

Reaction conditions: **1a** (0.3 mmol), **2a** (0.9 mmol), 4CzIPN(5 mol%) and DBU (2.0 equiv.) reacted in DCM (3.0 mL) at room temperature for 6 h under the irradiation of blue LED (20 W) in the O₂ atmosphere. ^[a] Isolated yields. ^[b] **2a** (0.6 mmol). ^[c] **2a** (0.75 mmol).

V. Unsuitable (hetero)aromatic cycles and amines.

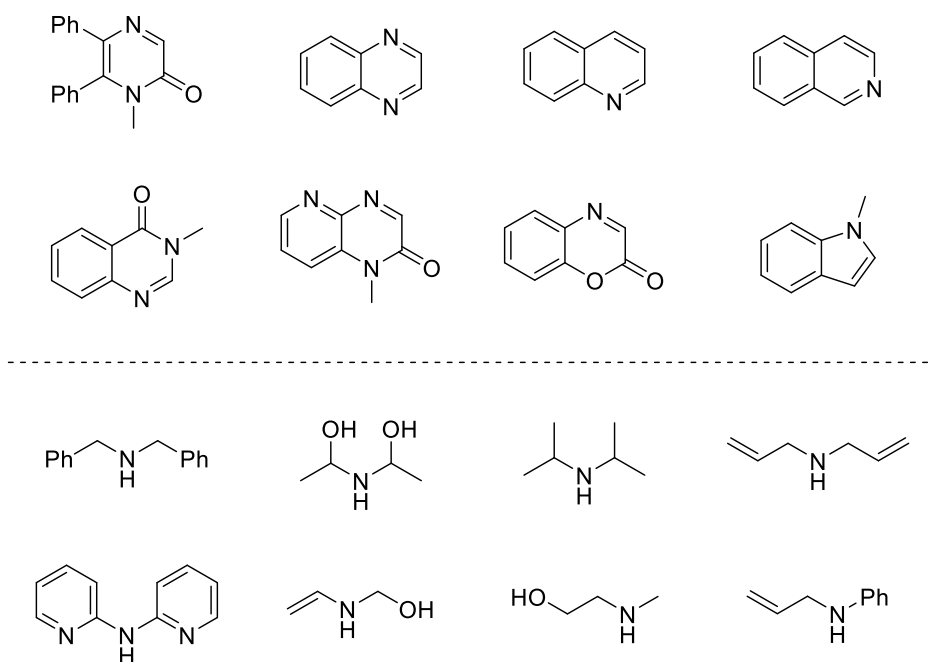


Figure S1 Unsuitable (hetero)aromatic cycles and amines

VI. Procedure for emission quenching experiments

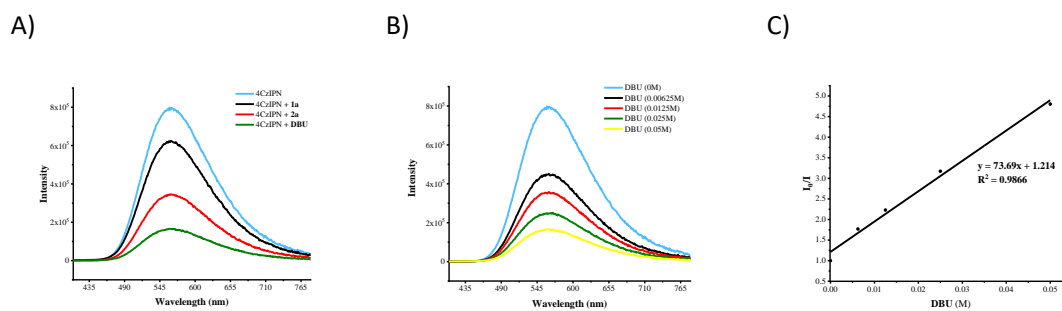


Figure S2 Luminescence quenching study

Emission intensities were recorded using an FS5 Spectrofluorometer. First, the emission intensity of 4CzIPN solutions was observed at 550 nm. The solutions were irradiated at 378 nm (Maximum absorption wavelength of 4CzIPN) and fluorescence was measured from 400 nm to 700 nm. In a typical experiment, the emission spectrum of a 5×10^{-5} M solution of 4CzIPN with different concentration of **1a**, **2a** and DBU in degassed anhydrous CH_3CN in 10 mm path length quartz cuvette was collected: A) the emission spectra of 5×10^{-5} M solutions of 4CzIPN with reactants (**1a**, **2a** and DBU) in degassed anhydrous CH_3CN ; B) the emission spectra of a 5×10^{-5} M solution of 4CzIPN with various concentrations of DBU in degassed anhydrous CH_3CN . C) the linear relationship between I_0/I

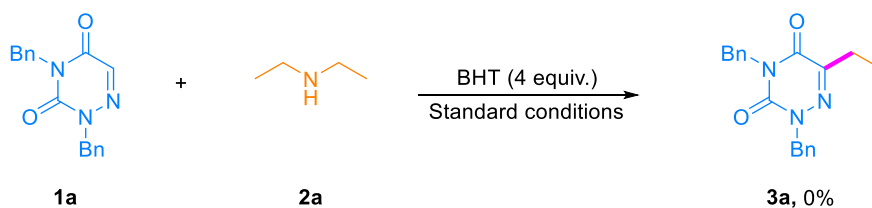
and the increasing concentration of DBU (I_0 and I are the fluorescence intensities before and after the increasing the concentration of DBU, respectively.).

VII. Mechanistic Experiments

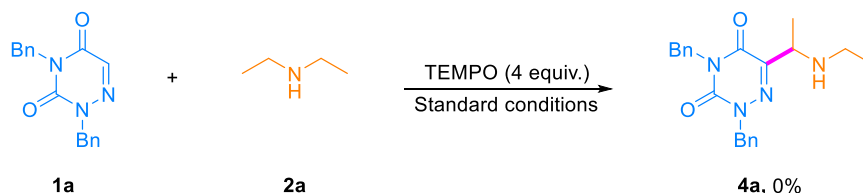
Control experiment



To a solution of 2,4-dibenzyl-1,2,4-triazine-3,5(*2H*, *4H*)-dione **1a** (0.3 mmol), 4CzIPN (5 mol%) and 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO) (4.0 equiv.) in DMC (3 mL) were placed in a flame-dried Schlenk-tube equipped with a magnetic stir bar, followed by addition of pyruvic acid (1.5 equiv.) and diethylamine **2a** (0.6 mmol) *via* syringe. The reaction was stirred at room temperature and irradiated with a 20 W blue light-emitting diode (LED) lamp for 12 h. The target product **3a** was not detected by TLC.

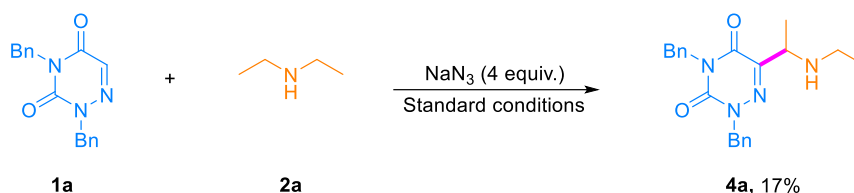


To a solution of 2,4-dibenzyl-1,2,4-triazine-3,5(*2H*, *4H*)-dione **1a** (0.3 mmol), 4CzIPN (5 mol%) and butylated hydroxytoluene (BHT) (4.0 equiv.) in DMC (3 mL) were placed in a flame-dried Schlenk-tube equipped with a magnetic stir bar, followed by addition of pyruvic acid (1.5 equiv.) and diethylamine **2a** (0.6 mmol) *via* syringe. The reaction was stirred at room temperature and irradiated with a 20 W blue light-emitting diode (LED) lamp for 12 h. The target product **3a** was not detected by TLC.



To a solution of 2,4-dibenzyl-1,2,4-triazine-3,5(*2H*, *4H*)-dione **1a** (0.3 mmol), 4CzIPN (5 mol%) and 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO) (4.0 equiv.) in DCM (3 mL) were placed in a flame-dried Schlenk-tube equipped with a magnetic stir bar, followed by addition of DBU (2.0 equiv.) and diethylamine **2a** (0.9 mmol) *via* syringe. The reaction was stirred at room temperature under O_2 atmosphere and irradiated with a 20 W blue light-emitting diode (LED) lamp for 6 h. The target

Schlenk-tube equipped with a magnetic stir bar, followed by addition of DBU (2.0 equiv.) and diethylamine **2a** (0.9 mmol) *via* syringe. The reaction was stirred at room temperature under O₂ atmosphere and irradiated with a 20 W blue light-emitting diode (LED) lamp for 6 h. The progress of the reaction was monitored by TLC. After completion, the reaction mixture was removed under reduced pressure. The crude residue thus obtained was purified by column chromatography over silica gel using petroleum ether and ethyl acetate (1:1) as an eluent to afford the 2,4-dibenzyl-6-(1-(ethylamino)ethyl)-1,2,4-triazine-3,5(2*H*, 4*H*)-dione **4a** in 24% yield.



To a solution of 2,4-dibenzyl-1,2,4-triazine-3,5(2*H*, 4*H*)-dione **1a** (0.3 mmol), 4CzIPN (5 mol%) and NaN₃ (4.0 equiv.) in DCM (3 mL) were placed in a flame-dried Schlenk-tube equipped with a magnetic stir bar, followed by addition of DBU (2.0 equiv.) and diethylamine **2a** (0.9 mmol) *via* syringe. The reaction was stirred at room temperature under O₂ atmosphere and irradiated with a 20 W blue light-emitting diode (LED) lamp for 6 h. The progress of the reaction was monitored by TLC. After completion, the reaction mixture was removed under reduced pressure. The crude residue thus obtained was purified by column chromatography over silica gel using petroleum ether and ethyl acetate (1:1) as an eluent to afford the 2,4-dibenzyl-6-(1-(ethylamino)ethyl)-1,2,4-triazine-3,5(2*H*, 4*H*)-dione **4a** in 17% yield.

VIII. Scale-up experiment

Gram-scale synthesis of **3a**

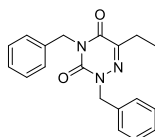
To a solution of 2,4-dibenzyl-1,2,4-triazine-3,5(2*H*, 4*H*)-dione **1a** (1.17 g, 4 mmol) and 4CzIPN (5 mol%) in DMC (0.1 M) were placed in a flame-dried Schlenk-tube equipped with a magnetic stir bar, followed by addition of pyruvic acid (1.5 equiv.) and diethylamine **2a** (0.59g, 8 mmol) *via* syringe. The reaction was stirred at room temperature and irradiated with a 20 W blue light-emitting diode (LED) lamp for 24 h. The progress of the reaction was monitored by TLC. After completion, the reaction mixture was removed under reduced pressure. The crude residue thus obtained was purified by column chromatography over silica gel using petroleum ether and ethyl acetate (25:1) as an eluent to afford the 2,4-dibenzyl-6-ethyl-1,2,4-triazine-3,5(2*H*, 4*H*)-dione **3a** (1.04 g) in 81% yield.

Gram-scale synthesis of **4a**

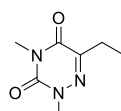
To a solution of 2,4-dibenzyl-1,2,4-triazine-3,5(2*H*, 4*H*)-dione **1a** (1.17 g, 4 mmol) and 4CzIPN (5 mol%) in DCM (0.1 M) were placed in a flame-dried Schlenk-tube equipped with a magnetic stir bar, followed by addition of DBU (2.0 equiv.) and diethylamine **2a** (0.88g, 12 mmol) *via* syringe. The reaction was stirred at room temperature under O₂ atmosphere and irradiated with a 20 W blue

light-emitting diode (LED) lamp for 6 h. The progress of the reaction was monitored by TLC. After completion, the reaction mixture was removed under reduced pressure. The crude residue thus obtained was purified by column chromatography over silica gel using petroleum ether and ethyl acetate (1:1) as an eluent to afford the 2,4-dibenzyl-6-(1-(ethylamino)ethyl)-1,2,4-triazine-3,5(2*H*, 4*H*)-dione **4a** (0.90 g) in 62% yield.

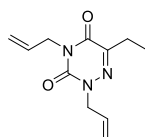
IX. Characterization data of 3a-4aa



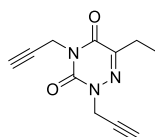
*2,4-dibenzyl-6-ethyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3a)*. a colorless liquid (91% yield, 87.3 mg). (PET/EtOAc = 25:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 7.49–7.48 (m, 2H), 7.42–7.41 (m, 2H), 7.37–7.30 (m, 6H), 5.09 (s, 2H), 5.09 (s, 2H), 2.64 (t, *J* = 7.4 Hz, 2H), 1.19 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 156.0, 149.1, 146.6, 136.0, 135.8, 129.5, 128.8, 128.7, 128.6, 128.2, 128.1, 55.3, 44.2, 23.9, 10.4; HRMS (ESI): *m/z* calcd for C₁₉H₂₀N₃O₂⁺ [M+H]⁺ 322.1550. Found 322.1550.



*6-ethyl-2,4-dimethyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3b)*. a colorless liquid (51% yield, 25.9 mg). (PET/EtOAc = 25:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 3.61 (s, 3H), 3.35 (s, 3H), 2.64 (q, *J* = 7.3 Hz, 2H), 1.19 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 156.4, 149.4, 145.8, 39.3, 27.1, 23.8, 10.6; HRMS (ESI): *m/z* calcd for C₇H₁₁N₃NaO₂⁺ [M+Na]⁺ 192.0743. Found 192.0743.

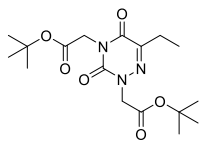


*2,4-diallyl-6-ethyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3c)*. a colorless liquid (81% yield, 53.5 mg). (PET/EtOAc = 25:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 5.98–5.81 (m, 2H), 5.31–5.21 (m, 4H), 4.53 (s, 4H), 2.63 (q, *J* = 7.3 Hz, 2H), 1.18 (t, *J* = 7.3 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 155.7, 148.5, 146.4, 131.6, 130.5, 119.0, 118.8, 53.9, 42.8, 23.8, 10.5; HRMS (ESI): *m/z* calcd for C₁₁H₁₅N₃NaO₂⁺ [M+Na]⁺ 244.1056. Found 244.1053.

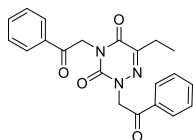


*6-ethyl-2,4-di(prop-2-yn-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (3d)*. a colorless liquid (87% yield, 56.8 mg). (PET/EtOAc = 25:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 4.74 (s, 2H), 4.68 (s, 2H), 2.68 (q, *J* = 7.3 Hz, 2H), 2.35 (s, 1H), 2.21 (s, 1H), 1.20 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 155.0, 147.6, 147.1, 76.9, 76.6, 73.3, 71.6, 41.2, 29.9, 23.8,

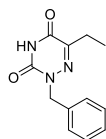
10.3; HRMS (ESI): m/z calcd for $C_{11}H_{11}N_3NaO_2^+$ $[M+Na]^+$ 240.0743. Found 240.0744.



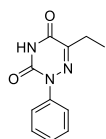
di-tert-butyl 2,2'-(6-ethyl-3,5-dioxo-1,2,4-triazine-2,4(3H,5H)-diyl)diacetate (3e). a colorless liquid (56% yield, 61.6 mg). (PET/EtOAc = 25:1 as the eluent). 1H NMR (400 MHz, $CDCl_3$) δ : 4.56 (s, 4H), 2.65 (q, $J = 7.0$ Hz, 2H), 1.46 (s, 18H), 1.17 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 166.5, 165.6, 155.5, 148.7, 146.6, 82.8, 82.7, 53.3, 42.0, 28.0, 27.9, 23.7, 10.3; HRMS (ESI): m/z calcd for $C_{17}H_{27}N_3NaO_6^+$ $[M+Na]^+$ 392.1792. Found 392.1794.



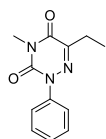
6-ethyl-2,4-bis(2-oxo-2-phenylethyl)-1,2,4-triazine-3,5(2H,4H)-dione (3f). a colorless liquid (73% yield, 82.6 mg). (PET/EtOAc = 25:1 as the eluent). 1H NMR (400 MHz, $CDCl_3$) δ : 7.98 (t, $J = 6.5$ Hz, 4H), 7.64–7.59 (m, 2H), 7.52–7.47 (m, 4H), 5.41 (s, 2H), 5.39 (s, 2H), 2.67 (q, $J = 7.3$ Hz, 2H), 1.19 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 191.6, 190.4, 155.7, 149.1, 146.8, 134.4, 134.3, 134.0, 133.9, 128.8, 128.7, 128.0, 127.9, 57.3, 46.4, 23.7, 10.2; HRMS (ESI): m/z calcd for $C_{21}H_{19}N_3NaO_4^+$ $[M+Na]^+$ 400.1268. Found 400.1264.



2-benzyl-6-ethyl-1,2,4-triazine-3,5(2H,4H)-dione (3g). a colorless liquid (89% yield, 61.7 mg). (PET/EtOAc = 25:1 as the eluent). 1H NMR (400 MHz, $CDCl_3$) δ : 9.92 (s, 1H), 7.50–7.48 (m, 2H), 7.34–7.28 (m, 3H), 5.09 (s, 2H), 2.63 (q, $J = 7.3$ Hz, 2H), 1.18 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 156.0, 150.1, 147.4, 135.4, 129.4, 128.6, 128.1, 43.5, 23.7, 10.2; HRMS (ESI): m/z calcd for $C_{12}H_{13}N_3NaO_2^+$ $[M+Na]^+$ 254.0900. Found 254.0899.

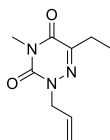


6-ethyl-2-phenyl-1,2,4-triazine-3,5(2H,4H)-dione (3h). a colorless liquid (31% yield, 20.1 mg). (PET/EtOAc = 25:1 as the eluent). 1H NMR (400 MHz, $CDCl_3$) δ : 10.21 (s, 1H), 7.56–7.47 (m, 3H), 7.27 (s, 2H), 2.70 (q, $J = 7.2$ Hz, 2H), 1.23 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 155.9, 150.0, 147.9, 132.3, 129.5, 129.4, 127.8, 23.8, 10.2; HRMS (ESI): m/z calcd for $C_{11}H_{11}N_3NaO_2^+$ $[M+Na]^+$ 240.0743. Found 240.0742.

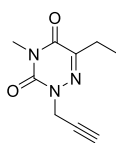


6-ethyl-4-methyl-2-phenyl-1,2,4-triazine-3,5(2H,4H)-dione (3i). a colorless liquid (79% yield, 54.8 mg). (PET/EtOAc = 25:1 as the eluent). 1H NMR (400 MHz, $CDCl_3$) δ : 7.52–7.43 (m, 3

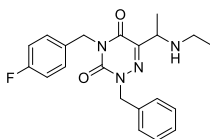
H), 7.23–7.21 (m, 2H), 3.66 (s, 3H), 2.69 (q, $J = 7.3$ Hz, 2H), 1.24 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 156.1, 149.0, 146.8, 133.2, 129.4, 129.2, 127.8, 39.4, 23.9, 10.5; HRMS (ESI): m/z calcd for $\text{C}_{12}\text{H}_{14}\text{N}_3\text{O}_2^+$ $[\text{M}+\text{H}]^+$ 232.1081. Found 232.1080.



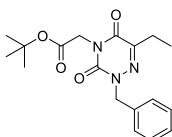
2-allyl-6-ethyl-4-methyl-1,2,4-triazine-3,5(2H,4H)-dione (3j). a colorless liquid (79% yield, 46.5 mg). (PET/EtOAc = 25:1 as the eluent). ^1H NMR (400 MHz, CDCl_3) δ : 5.90–5.81 (m, 1H), 5.31–5.21 (m, 2H), 4.52 (d, $J = 5.5$ Hz, 2H), 3.60 (s, 3H), 2.63 (q, $J = 7.3$ Hz, 2H), 1.18 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 155.9, 148.9, 146.1, 130.5, 119.1, 42.8, 39.2, 23.7, 10.5; HRMS (ESI): m/z calcd for $\text{C}_9\text{H}_{13}\text{N}_3\text{NaO}_2^+$ $[\text{M}+\text{Na}]^+$ 218.0900. Found 218.0903.



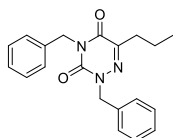
6-ethyl-4-methyl-2-(prop-2-yn-1-yl)-1,2,4-triazine-3,5(2H,4H)-dione (3k). a colorless liquid (85% yield, 49.3 mg). (PET/EtOAc = 25:1 as the eluent). ^1H NMR (400 MHz, CDCl_3) δ : 4.68–4.67 (m, 2H), 3.61 (s, 3H), 2.64 (q, $J = 7.3$ Hz, 2H), 2.20 (s, 1H), 1.18 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 155.2, 148.3, 146.1, 76.8, 71.4, 39.3, 29.8, 23.7, 10.4; HRMS (ESI): m/z calcd for $\text{C}_9\text{H}_{11}\text{N}_3\text{NaO}_2^+$ $[\text{M}+\text{Na}]^+$ 216.0743. Found 216.0742.



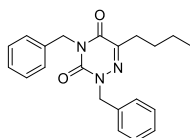
2-benzyl-6-(1-(ethylamino)ethyl)-4-(4-fluorobenzyl)-1,2,4-triazine-3,5(2H,4H)-dione (3l). a colorless liquid (65% yield, 65.8 mg). (PET/EtOAc = 25:1 as the eluent). ^1H NMR (400 MHz, CDCl_3) δ : 7.49–7.47 (m, 2H), 7.42–7.39 (m, 2H), 7.33–7.30 (m, 3H), 7.03 (t, $J = 8.4$ Hz, 2H), 5.08 (s, 2H), 5.05 (s, 2H), 2.64 (q, $J = 7.3$ Hz, 2H), 1.19 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 163.8, 161.4, 155.9, 149.0, 146.6, 135.6, 131.7, 130.7, 130.6, 129.4, 128.5, 128.0, 115.6, 115.4, 54.4, 44.1, 23.7, 10.3; HRMS (ESI): m/z calcd for $\text{C}_{19}\text{H}_{18}\text{FN}_3\text{NaO}_2^+$ $[\text{M}+\text{Na}]^+$ 362.1275. Found 362.1274.



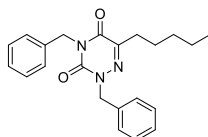
tert-butyl 2-(2-benzyl-6-ethyl-3,5-dioxo-2,5-dihydro-1,2,4-triazin-4(3H)-yl)acetate (3m). a colorless liquid (76% yield, 79.0 mg). (PET/EtOAc = 25:1 as the eluent). ^1H NMR (400 MHz, CDCl_3) δ : 7.47–7.45 (m, 2H), 7.30–7.28 (m, 2H), 5.10 (s, 2H), 4.56 (s, 2H), 2.64 (q, $J = 7.3$ Hz, 2H), 1.45 (s, 9H), 1.17 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 166.6, 155.9, 149.2, 146.8, 135.5, 129.2, 128.5, 127.9, 82.8, 53.3, 44.0, 27.9, 23.7, 10.3; HRMS (ESI): m/z calcd for $\text{C}_{18}\text{H}_{23}\text{N}_3\text{NaO}_4^+$ $[\text{M}+\text{Na}]^+$ 368.1581. Found 368.1578.



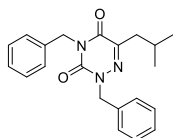
2,4-dibenzyl-6-propyl-1,2,4-triazine-3,5(2H,4H)-dione (3n). a colorless liquid (51% yield, 51.7 mg). ¹H NMR (400 MHz, CDCl₃) δ: 7.49–7.48 (m, 2H), 7.42–7.40 (m, 2H), 7.37–7.30 (m, 6H), 5.09 (s, 4H), 2.59 (t, *J* = 7.4 Hz, 2H), 1.69–1.63 (m, 2H), 0.97 (t, *J* = 7.3 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 156.0, 149.0, 145.6, 135.8, 135.7, 129.4, 128.6, 128.5, 128.1, 128.0, 55.1, 44.1, 32.2, 19.6, 13.7; HRMS (ESI): *m/z* calcd for C₂₀H₂₁N₃NaO₂⁺ [M+Na]⁺ 358.1526. Found 358.1524.



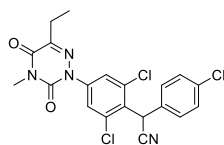
2,4-dibenzyl-6-butyl-1,2,4-triazine-3,5(2H,4H)-dione (3o). a colorless liquid (46% yield, 48.3 mg). (PET/EtOAc = 25:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 7.50–7.48 (m, 2H), 7.42–7.40 (m, 2H), 7.37–7.30 (m, 6H), 5.09 (s, 4H), 2.61 (t, *J* = 7.6 Hz, 2H), 1.63–1.57 (m, 2H), 1.38 (q, *J* = 7.3 Hz, 2H), 0.94 (t, *J* = 7.3 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 156.0, 149.0, 145.7, 135.8, 135.7, 129.4, 128.6, 128.6, 128.5, 128.1, 128.0, 55.1, 44.1, 30.0, 28.2, 22.2, 13.8; HRMS (ESI): *m/z* calcd for C₂₁H₂₃N₃NaO₂⁺ [M+Na]⁺ 372.1682. Found 372.1681.



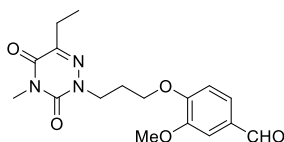
2,4-dibenzyl-6-pentyl-1,2,4-triazine-3,5(2H,4H)-dione (3p). a colorless liquid (34% yield, 37.2 mg). ¹H NMR (400 MHz, CDCl₃) δ: 7.50–7.48 (m, 2H), 7.42–7.40 (m, 2H), 7.37–7.30 (m, 6H), 5.09 (s, 4H), 2.61 (t, *J* = 7.6 Hz, 2H), 1.65–1.61 (m, 2H), 1.34 (s, 4H), 0.90 (t, *J* = 6.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 156.0, 149.0, 145.7, 135.9, 135.7, 129.4, 128.6, 128.6, 128.5, 128.1, 127.9, 55.1, 44.1, 31.3, 30.2, 25.8, 22.3, 14.0; HRMS (ESI): *m/z* calcd for C₂₂H₂₅N₃NaO₂⁺ [M+Na]⁺ 386.1839. Found 386.1839.



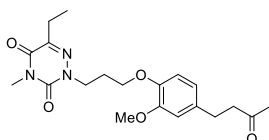
2,4-dibenzyl-6-isobutyl-1,2,4-triazine-3,5(2H,4H)-dione (3q). a colorless liquid (72% yield, 75.1 mg). (PET/EtOAc = 25:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 7.48–7.47 (m, 2H), 7.41–7.39 (m, 2H), 7.34–7.30 (m, 6H), 5.09 (s, 2H), 5.09 (s, 2H), 2.48 (d, *J* = 7.0 Hz, 2H), 2.13–2.03 (m, 1H), 0.93 (d, *J* = 6.6 Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) δ: 156.1, 148.9, 145.0, 135.8, 135.7, 129.4, 128.6, 128.6, 128.5, 128.1, 128.0, 55.2, 44.1, 39.0, 26.2, 22.4; HRMS (ESI): *m/z* calcd for C₂₁H₂₃N₃NaO₂⁺ [M+Na]⁺ 372.1682. Found 372.1682.



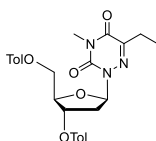
2-(4-chlorophenyl)-2-(2,6-dichloro-4-(6-ethyl-4-methyl-3,5-dioxo-4,5-dihydro-1,2,4-triazin-2(3H)-yl)phenyl)acetonitrile (**3r**), a colorless liquid (41% yield, 55.1 mg). (PET/EtOAc = 25:1 as the eluet). ¹H NMR (400 MHz, CDCl₃) δ: 7.79 (s, 2H), 7.33 (q, *J* = 8.2 Hz, 4H), 6.18 (s, 1H), 3.42 (s, 3H), 2.77 (q, *J* = 7.1 Hz, 2H), 1.26 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 155.3, 148.2, 141.7, 135.6, 134.2, 130.8, 129.6, 129.1, 128.2, 124.8, 116.2, 36.9, 27.5, 24.1, 10.4; HRMS (ESI): *m/z* calcd for C₂₀H₁₅C₁₃N₄NaO₂⁺ [M+Na]⁺ 471.0153. Found 471.0153.



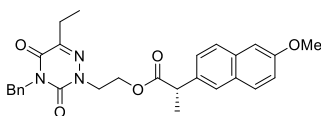
4-(3-(6-ethyl-4-methyl-3,5-dioxo-4,5-dihydro-1,2,4-triazin-2(3H)-yl)propoxy)-3-methoxybenzaldehyde (**3s**), a colorless liquid (37% yield, 43.0 mg). (PET/EtOAc = 25:1 as the eluet). ¹H NMR (400 MHz, CDCl₃) δ: 9.83 (s, 1H), 7.41 (d, *J* = 7.7 Hz, 1H), 7.36 (s, 1H), 6.91 (d, *J* = 8.2 Hz, 1H), 4.21–4.17 (m, 4H), 3.83 (s, 3H), 3.54 (s, 3H), 2.57 (q, *J* = 7.2 Hz, 2H), 2.28–2.26 (m, 2H), 1.15 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 190.9, 156.4, 153.6, 149.6, 149.3, 145.9, 130.0, 127.0, 111.2, 108.8, 67.4, 55.7, 38.8, 29.7, 27.0, 23.7, 10.4; HRMS (ESI): *m/z* calcd for C₁₇H₂₁N₃NaO₅⁺ [M+Na]⁺ 370.1373. Found 370.1371.



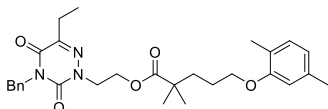
6-ethyl-2-(3-(2-methoxy-4-(3-oxobutyl)phenoxy)propyl)-4-methyl-1,2,4-triazine-3,5-dione (**3t**), a colorless liquid (40% yield, 51.9 mg). (PET/EtOAc = 25:1 as the eluet). ¹H NMR (400 MHz, CDCl₃) δ: 6.76–6.74 (m, 1H), 6.66 (s, 2H), 4.15 (t, *J* = 6.5 Hz, 2H), 4.05 (t, *J* = 5.8 Hz, 2H), 3.78 (s, 3H), 3.56 (s, 3H), 2.83–2.80 (m, 2H), 2.74–2.70 (m, 2H), 2.58 (q, *J* = 7.2 Hz, 2H), 2.20–2.17 (m, 2H), 2.13 (s, 3H), 1.15 (t, *J* = 7.3 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 208.1, 156.3, 149.3, 149.2, 146.5, 145.9, 133.9, 120.1, 113.4, 112.1, 67.2, 55.7, 45.4, 39.2, 38.7, 30.1, 29.4, 27.2, 23.7, 10.4; HRMS (ESI): *m/z* calcd for C₂₀H₂₇N₃NaO₅⁺ [M+Na]⁺ 412.1843. Found 412.1844.



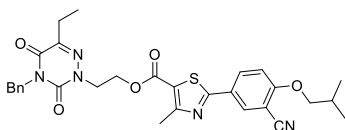
(2*R*,3*S*,5*R*)-5-(6-ethyl-4-methyl-3,5-dioxo-4,5-dihydro-1,2,4-triazin-2(3H)-yl)-2-(((4-methylbenzoyl)oxy)methyl)tetrahydrofuran-3-yl 4-methylbenzoate (**3u**), a colorless liquid (51% yield, 77.6 mg). (PET/EtOAc = 25:1 as the eluet). ¹H NMR (400 MHz, CDCl₃) δ: 7.92 (t, *J* = 9.2 Hz, 4H), 7.26–7.24 (m, 2H), 7.19 (d, *J* = 7.6 Hz, 2H), 6.75–6.72 (m, 1H), 5.74 (s, 1H), 4.58–4.55 (m, 1H), 4.53–4.49 (m, 1H), 3.34 (s, 3H), 3.06–2.99 (m, 1H), 2.65 (q, *J* = 7.1 Hz, 2H), 2.49–2.39 (m, 8H), 1.21 (t, *J* = 7.3 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 166.2, 166.0, 155.7, 149.3, 147.1, 144.2, 143.8, 129.7, 129.7, 129.2, 129.0, 126.9, 126.6, 86.5, 81.9, 75.0, 64.4, 34.9, 27.2, 24.0, 21.7, 21.6, 10.3; HRMS (ESI): *m/z* calcd for C₂₇H₂₉N₃NaO₇⁺ [M+Na]⁺ 530.1898. Found 530.1894.



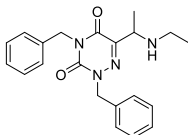
2-(4-benzyl-6-ethyl-3,5-dioxo-4,5-dihydro-1,2,4-triazin-2(3H)-yl)ethyl (S)-2-(6-methoxynaphthalen-2-yl)propanoate (**3v**). a colorless liquid (37% yield, 54.1 mg). (PET/EtOAc = 25:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 7.68–7.63 (m, 2H), 7.58 (s, 1H), 7.40–7.31 (m, 6H), 7.14–7.10 (m, 2H), 4.99 (s, 2H), 4.45–4.38 (m, 1H), 4.31–4.21 (m, 2H), 4.16–4.09 (m, 1H), 3.91 (s, 3H), 3.72 (q, *J* = 7.2 Hz, 1H), 2.54 (q, *J* = 7.4 Hz, 2H), 3.72 (d, *J* = 7.1 Hz, 3H), 1.16 (t, *J* = 7.3 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 174.4, 157.6, 155.9, 148.8, 146.1, 135.9, 135.4, 133.6, 129.2, 128.8, 128.7, 128.6, 128.1, 127.0, 126.2, 125.9, 118.9, 105.5, 61.0, 55.3, 55.1, 45.3, 39.6, 23.6, 18.4, 10.3; HRMS (ESI): *m/z* calcd for C₂₈H₃₀N₃O₅⁺ [M+H]⁺ 488.2180. Found 488.2176.



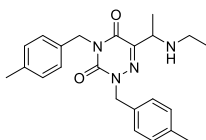
2-(4-benzyl-6-ethyl-3,5-dioxo-4,5-dihydro-1,2,4-triazin-2(3H)-yl)ethyl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (**3w**). a colorless liquid (43% yield, 65.4 mg). (PET/EtOAc = 25:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 7.40–7.39 (m, 2H), 7.35–7.31 (m, 3H), 7.00 (d, *J* = 7.0 Hz, 1H), 6.65 (d, *J* = 7.2 Hz, 1H), 6.59 (s, 1H), 5.08 (s, 2H), 4.32–4.31 (m, 2H), 4.24–4.23 (m, 2H), 3.88–3.85 (m, 2H), 2.63 (q, *J* = 7.2 Hz, 2H), 2.31 (s, 3H), 2.16 (s, 3H), 1.66–1.65 (m, 2H), 1.28 (d, *J* = 10.7 Hz, 2H), 1.20–1.17 (m, 3H), 1.13 (s, 6H); ¹³C NMR (100 MHz, CDCl₃) δ: 177.6, 157.0, 156.1, 148.9, 146.3, 136.5, 135.9, 130.3, 128.8, 128.7, 128.2, 123.6, 120.7, 112.0, 67.9, 60.8, 55.2, 42.0, 39.8, 36.9, 29.8, 25.1, 25.0, 23.9, 21.5, 15.8, 10.5; HRMS (ESI): *m/z* calcd for C₂₉H₃₈N₃O₅⁺ [M+H]⁺ 508.2806. Found 508.2805.



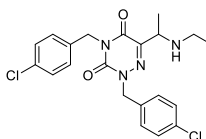
2-(4-benzyl-6-ethyl-3,5-dioxo-4,5-dihydro-1,2,4-triazin-2(3H)-yl)ethyl 2-(3-cyano-4-isobutoxyphenyl)-4-methylthiazole-5-carboxylate (**3x**). a colorless liquid (19% yield, 32.7 mg). (PET/EtOAc = 25:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 8.13 (s, 1H), 8.07 (d, *J* = 8.8 Hz, 1H), 8.38–7.34 (m, 3H), 7.30–7.27 (m, 2H), 7.01 (d, *J* = 8.9 Hz, 1H), 5.09 (s, 2H), 4.55–4.53 (m, 2H), 4.36–4.34 (m, 2H), 3.91–3.90 (m, 2H), 2.70 (s, 3H), 2.64 (q, *J* = 7.3 Hz, 2H), 2.24–2.18 (m, 1H), 1.18 (t, *J* = 7.4 Hz, 3H), 1.10 (t, *J* = 6.7 Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) δ: 167.5, 162.5, 161.7, 161.7, 156.0, 148.9, 146.4, 135.7, 132.6, 132.1, 128.6, 128.1, 126.0, 121.1, 115.4, 112.6, 103.0, 75.7, 61.6, 55.1, 39.7, 28.1, 23.9, 19.0, 17.4, 10.4; HRMS (ESI): *m/z* calcd for C₃₀H₃₂N₅O₅S⁺ [M+H]⁺ 574.2119. Found 574.2119.



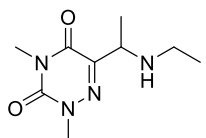
2,4-dibenzyl-6-(1-(ethylamino)ethyl)-1,2,4-triazine-3,5(2H,4H)-dione (**4a**). a yellow liquid (79% yield, 86.3 mg). (PET/EtOAc = 1:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 7.48–7.46 (m, 2H), 7.40–7.38 (m, 2H), 7.34–7.30 (m, 6H), 5.18–5.02 (m, 4H), 3.98 (q, *J* = 6.4 Hz, 1H), 2.52–2.51 (m, 2H), 1.84 (s, 1H), 1.36 (d, *J* = 6.6 Hz, 3H), 1.06 (t, *J* = 7.0 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 155.4, 148.7, 146.8, 135.6, 135.5, 129.3, 128.6, 128.6, 128.5, 128.2, 128.0, 55.2, 53.3, 44.0, 41.4, 19.6, 15.3; HRMS (ESI): *m/z* calcd for C₂₁H₂₅N₄O₂⁺ [M+H]⁺ 365.1972. Found 365.1972.



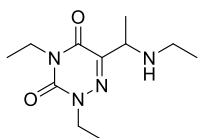
6-(1-(ethylamino)ethyl)-2,4-bis(4-methylbenzyl)-1,2,4-triazine-3,5(2H,4H)-dione (**4b**). a yellow liquid (74% yield, 86.9 mg). (PET/EtOAc = 1:1 as the eluet). ^1H NMR (400 MHz, CDCl_3) δ : 7.38–7.36 (m, 2H), 7.29–7.26 (m, 2H), 7.13 (t, J = 8.1 Hz, 4H), 5.13–4.98 (m, 4H), 3.96 (q, J = 6.4 Hz, 1H), 2.51 (q, J = 6.8 Hz, 2H), 2.33 (s, 3H), 2.32 (s, 3H), 1.87 (s, 1H), 1.34 (d, J = 6.4 Hz, 3H), 1.06 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 155.5, 148.7, 146.6, 137.9, 137.8, 132.6, 129.4, 129.3, 129.2, 128.6, 55.0, 53.3, 43.8, 41.4, 21.1, 19.6, 15.2; HRMS (ESI): m/z calcd for $\text{C}_{23}\text{H}_{29}\text{N}_4\text{O}_2^+$ $[\text{M}+\text{H}]^+$ 393.2285. Found 393.2284.



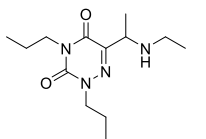
2,4-bis(4-chlorobenzyl)-6-(1-(ethylamino)ethyl)-1,2,4-triazine-3,5(2H,4H)-dione (**4c**). a yellow liquid (64% yield, 82.6 mg). (PET/EtOAc = 1:1 as the eluet). ^1H NMR (400 MHz, CDCl_3) δ : 7.41–7.39 (m, 2H), 7.31–7.27 (m, 6H), 5.12–4.99 (m, 4H), 3.96 (q, J = 6.6 Hz, 1H), 2.58–2.47 (m, 2H), 1.83 (s, 1H), 1.35 (d, J = 6.7 Hz, 3H), 1.07 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 155.3, 148.6, 147.1, 134.3, 134.1, 133.9, 133.9, 130.9, 130.1, 128.9, 128.7, 54.6, 53.3, 43.4, 41.5, 19.5, 15.3; HRMS (ESI): m/z calcd for $\text{C}_{21}\text{H}_{23}\text{Cl}_2\text{N}_4\text{O}_2^+$ $[\text{M}+\text{H}]^+$ 433.1193. Found 433.1190.



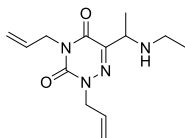
6-(1-(ethylamino)ethyl)-2,4-dimethyl-1,2,4-triazine-3,5(2H,4H)-dione (**4d**). a yellow liquid (74% yield, 47.2 mg). (PET/EtOAc = 1:1 as the eluet). ^1H NMR (400 MHz, CDCl_3) δ : 3.99 (q, J = 6.5 Hz, 1H), 3.61 (s, 3H), 3.32 (s, 3H), 2.89 (s, 1H), 2.62–2.60 (m, 2H), 1.38 (d, J = 6.5 Hz, 3H), 1.11 (t, J = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 155.8, 149.0, 145.2, 53.3, 41.5, 39.5, 27.0, 19.1, 14.8; HRMS (ESI): m/z calcd for $\text{C}_9\text{H}_{17}\text{N}_4\text{O}_2^+$ $[\text{M}+\text{H}]^+$ 213.1346. Found 213.1345.



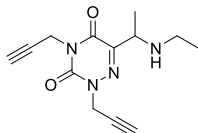
2,4-diethyl-6-(1-(ethylamino)ethyl)-1,2,4-triazine-3,5(2H,4H)-dione (**4e**). a yellow liquid (65% yield, 47.3 mg). (PET/EtOAc = 1:1 as the eluet). ^1H NMR (400 MHz, CDCl_3) δ : 4.04–3.99 (m, 1H), 3.97–3.93 (m, 4H), 2.59–2.54 (m, 2H), 1.94 (s, 1H), 1.35 (d, J = 6.7 Hz, 3H), 1.30 (t, J = 7.1 Hz, 3H), 1.22 (t, J = 7.0 Hz, 3H), 1.08 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 155.4, 148.3, 146.2, 53.4, 46.7, 41.5, 36.0, 19.4, 15.2, 13.3, 12.5; HRMS (ESI): m/z calcd for $\text{C}_{11}\text{H}_{21}\text{N}_4\text{O}_2^+$ $[\text{M}+\text{H}]^+$ 241.1659. Found 241.1658.



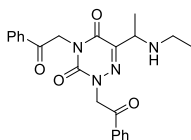
6-(1-(ethylamino)ethyl)-2,4-dipropyl-1,2,4-triazine-3,5(2H,4H)-dione (**4f**). a yellow liquid (68% yield, 54.6 mg). (PET/EtOAc = 1:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 3.95-3.91 (m, 1H), 3.89-3.83 (m, 4H), 2.54 (q, *J* = 6.6 Hz, 2H), 2.02 (s, 1H), 1.73 (t, *J* = 7.3 Hz, 2H), 1.63 (t, *J* = 7.4 Hz, 2H), 1.31 (d, *J* = 6.7 Hz, 3H), 1.06 (t, *J* = 7.1 Hz, 3H), 0.91 (t, *J* = 7.4 Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) δ: 155.5, 148.7, 146.1, 53.4, 53.0, 42.2, 41.4, 21.4, 20.5, 19.4, 15.3, 11.2, 10.8; HRMS (ESI): *m/z* calcd for C₁₃H₂₅N₄O₂⁺ [M+H]⁺ 269.1972. Found 269.1973.



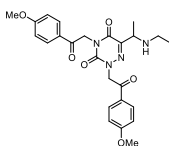
2,4-diallyl-6-(1-(ethylamino)ethyl)-1,2,4-triazine-3,5(2H,4H)-dione (**4g**). a yellow liquid (63% yield, 49.7 mg). (PET/EtOAc = 1:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 5.96-5.80 (m, 2H), 5.29-5.20 (m, 4H), 4.60-4.50 (m, 4H), 3.95 (q, *J* = 6.4 Hz, 1H), 2.58-2.53 (m, 2H), 1.90 (s, 1H), 1.35 (d, *J* = 6.7 Hz, 3H), 1.07 (t, *J* = 7.0 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 155.2, 148.3, 146.7, 131.3, 130.3, 119.1, 118.9, 53.9, 53.5, 42.8, 41.5, 19.5, 15.3; HRMS (ESI): *m/z* calcd for C₁₃H₂₁N₄O₂⁺ [M+H]⁺ 265.1659. Found 265.1661.



6-(1-(ethylamino)ethyl)-2,4-di(prop-2-yn-1-yl)-1,2,4-triazine-3,5(2H,4H)-dione (**4h**). a yellow liquid (66% yield, 51.4 mg). (PET/EtOAc = 1:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 4.80-4.68 (m, 4H), 3.99 (q, *J* = 6.1 Hz, 1H), 2.59 (q, *J* = 6.7 Hz, 2H), 2.35 (s, 1H), 2.22 (s, 1H), 1.83 (s, 1H), 1.39 (d, *J* = 6.6 Hz, 3H), 1.09 (t, *J* = 6.9 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 154.5, 147.5, 147.4, 76.4, 73.5, 71.8, 53.5, 41.5, 41.3, 29.9, 19.5, 15.3; HRMS (ESI): *m/z* calcd for C₁₃H₁₇N₄O₂⁺ [M+H]⁺ 261.1346. Found 261.1341.

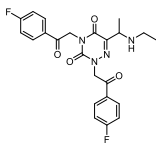


6-(1-(ethylamino)ethyl)-2,4-bis(2-oxo-2-phenylethyl)-1,2,4-triazine-3,5(2H,4H)-dione (**4i**). a yellow liquid (66% yield, 83.7 mg). (PET/EtOAc = 1:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 7.99-7.95 (m, 4H), 7.64-7.59 (m, 2H), 7.51-7.47 (m, 4H), 5.43-5.38 (m, 4H), 4.00 (q, *J* = 6.7 Hz, 1H), 2.65-2.56 (m, 2H), 2.17 (s, 1H), 1.39 (d, *J* = 6.7 Hz, 3H), 1.08 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 191.5, 190.3, 155.3, 148.9, 147.3, 134.4, 134.3, 134.1, 134.0, 128.9, 128.8, 128.1, 128.0, 57.4, 53.5, 46.4, 41.4, 19.5, 15.3; HRMS (ESI): *m/z* calcd for C₂₃H₂₅N₄O₄⁺ [M+H]⁺ 421.1870. Found 421.1870.

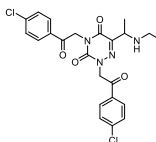


6-(1-(ethylamino)ethyl)-2,4-bis(2-(4-methoxyphenyl)-2-oxoethyl)-1,2,4-triazine-3,5(2H,4H)-dione (**4j**). a yellow liquid (64% yield, 92.0 mg). (PET/EtOAc = 1:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 7.97-7.92 (m, 4H), 6.96-6.94 (m, 4H), 5.37-5.33 (m, 4H), 3.99 (q, *J* = 6.3 Hz, 1H), 3.86 (s, 6H),

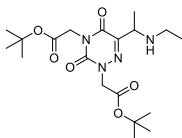
2.65-2.55 (m, 2H), 2.06 (s, 1H), 1.39 (d, $J = 6.6$ Hz, 3H), 1.07 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 190.0, 188.8, 164.3, 155.4, 149.1, 147.2, 130.5, 130.4, 127.6, 127.4, 114.2, 114.1, 57.2, 55.6, 53.6, 46.2, 41.5, 19.6, 15.4; HRMS (ESI): m/z calcd for $\text{C}_{25}\text{H}_{29}\text{N}_4\text{O}_6^+$ $[\text{M}+\text{H}]^+$ 481.2082. Found 481.2076.



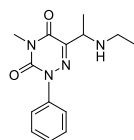
6-(1-(ethylamino)ethyl)-2,4-bis(2-(4-fluorophenyl)-2-oxoethyl)-1,2,4-triazine-3,5(2H,4H)-dione (**4k**). a yellow liquid (62% yield, 85.3 mg). (PET/EtOAc = 1:1 as the eluet). ^1H NMR (400 MHz, CDCl_3) δ : 8.03-7.97 (m, 4H), 7.19-7.14 (m, 4H), 5.39-5.34 (m, 4H), 3.99 (q, $J = 6.3$ Hz, 1H), 2.61-2.58 (m, 2H), 2.19 (s, 1H), 1.38 (d, $J = 6.6$ Hz, 3H), 1.07 (t, $J = 6.9$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 189.9, 188.7, 167.5, 167.5, 164.9, 164.9, 155.2, 148.9, 147.3, 130.8(d, $J = 9.6$ Hz), 116.2(d, $J = 8.3$ Hz), 116.0(d, $J = 8.4$ Hz), 57.2, 53.5, 46.2, 41.4, 19.5, 15.2; HRMS (ESI): m/z calcd for $\text{C}_{23}\text{H}_{23}\text{F}_2\text{N}_4\text{O}_4^+$ $[\text{M}+\text{H}]^+$ 457.1682. Found 457.1681.



2,4-bis(2-(4-chlorophenyl)-2-oxoethyl)-6-(1-(ethylamino)ethyl)-1,2,4-triazine-3,5(2H,4H)-dione (**4l**). a yellow liquid (61% yield, 89.7 mg). (PET/EtOAc = 1:1 as the eluet). ^1H NMR (400 MHz, CDCl_3) δ : 7.94-7.89 (m, 4H), 7.49-7.47 (m, 4H), 5.39-5.34 (m, 4H), 4.00 (q, $J = 6.5$ Hz, 1H), 2.64-2.57 (m, 2H), 1.79 (s, 1H), 1.39 (d, $J = 6.7$ Hz, 3H), 1.08 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 190.3, 189.2, 155.2, 148.9, 147.5, 140.7, 140.7, 132.7, 132.6, 129.5, 129.4, 129.3, 129.3, 57.3, 53.6, 46.3, 41.5, 19.6, 15.3; HRMS (ESI): m/z calcd for $\text{C}_{23}\text{H}_{23}\text{Cl}_2\text{N}_4\text{O}_4^+$ $[\text{M}+\text{H}]^+$ 489.1091. Found 489.1083.

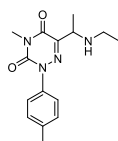


di-tert-butyl 2,2'-(6-(1-(ethylamino)ethyl)-3,5-dioxo-1,2,4-triazine-2,4(3H,5H)-diyl)diacetate (**4m**). a yellow liquid (41% yield, 50.9 mg). (PET/EtOAc = 1:1 as the eluet). ^1H NMR (400 MHz, CDCl_3) δ : 4.62-4.54 (m, 4H), 4.00 (q, $J = 6.5$ Hz, 1H), 2.60-2.51 (m, 2H), 1.85 (s, 1H), 1.44 (s, 18H), 1.35 (d, $J = 6.5$ Hz, 3H), 1.06 (t, $J = 6.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 166.2, 165.4, 155.0, 148.5, 147.0, 82.9, 82.8, 53.5, 53.3, 42.0, 41.4, 27.9, 27.9, 19.6, 15.2; HRMS (ESI): m/z calcd for $\text{C}_{19}\text{H}_{33}\text{N}_4\text{O}_6^+$ $[\text{M}+\text{H}]^+$ 413.2395. Found 413.2394.

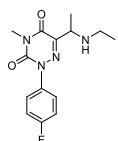


6-(1-(ethylamino)ethyl)-4-methyl-2-phenyl-1,2,4-triazine-3,5(2H,4H)-dione (**4n**). a yellow liquid (71% yield, 58.4 mg). (PET/EtOAc = 1:1 as the eluet). ^1H NMR (400 MHz, CDCl_3) δ : 7.51-7.43 (m, 3H), 7.22-7.20(m, 2H), 4.00 (q, $J = 6.3$ Hz, 1H), 3.66 (s, 3H), 2.66-2.63 (m, 2H), 1.93 (s, 1H), 1.39 (d, $J = 6.3$ Hz, 3H), 1.11 (t, $J = 6.6$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 155.6, 148.7, 146.9, 132.9, 129.5, 129.3, 127.7, 53.6, 41.5, 39.5, 19.3, 15.2; HRMS (ESI): m/z calcd for $\text{C}_{14}\text{H}_{19}\text{N}_4\text{O}_2^+$ $[\text{M}+\text{H}]^+$

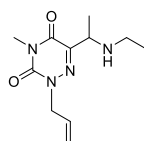
275.1503. Found 275.1504.



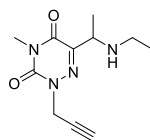
6-(1-(ethylamino)ethyl)-4-methyl-2-(p-tolyl)-1,2,4-triazine-3,5(2H,4H)-dione (**4o**). a yellow liquid (77% yield, 66.3 mg). (PET/EtOAc = 1:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 7.31-7.29 (m, 2H), 7.10-7.08 (m, 2H), 3.99 (q, *J* = 6.6 Hz, 1H), 3.66 (s, 3H), 2.65-2.63 (m, 2H), 2.39 (s, 3H), 1.94 (s, 1H), 1.40 (d, *J* = 6.7 Hz, 3H), 1.11 (t, *J* = 6.9 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 155.7, 148.7, 147.0, 139.4, 130.2, 130.1, 127.4, 53.6, 41.5, 39.5, 21.2, 19.3, 15.3; HRMS (ESI): *m/z* calcd for C₁₅H₂₁N₄O₂⁺ [M+H]⁺ 289.1659. Found 289.1653.



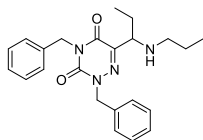
6-(1-(ethylamino)ethyl)-2-(4-fluorophenyl)-4-methyl-1,2,4-triazine-3,5(2H,4H)-dione (**4p**). a yellow liquid (56% yield, 48.7 mg). (PET/EtOAc = 1:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 7.20-7.18 (m, 4H), 3.99 (q, *J* = 6.6 Hz, 1H), 3.66 (s, 3H), 2.68-2.59 (m, 2H), 1.82 (s, 1H), 1.40 (d, *J* = 6.6 Hz, 3H), 1.11 (t, *J* = 7.0 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 163.9, 161.4, 155.6, 148.7, 147.1, 129.7 (d, *J* = 8.9 Hz), 128.6 (d, *J* = 3.2 Hz), 116.6, 116.4, 53.6, 41.6, 39.5, 19.4, 15.3; HRMS (ESI): *m/z* calcd for C₁₄H₁₈FN₄O₂⁺ [M+H]⁺ 293.1408. Found 293.1408.



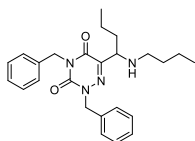
2-allyl-6-(1-(ethylamino)ethyl)-4-methyl-1,2,4-triazine-3,5(2H,4H)-dione (**4q**). a yellow liquid (64% yield, 45.6 mg). (PET/EtOAc = 1:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 5.90-5.81 (m, 1H), 5.31-5.22 (m, 2H), 4.53 (d, *J* = 5.5 Hz, 2H), 3.96 (q, *J* = 6.6 Hz, 1H), 3.62 (s, 3H), 2.63-2.54 (m, 2H), 1.78 (s, 1H), 1.36 (d, *J* = 6.6 Hz, 3H), 1.09 (t, *J* = 7.0 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 155.4, 148.7, 146.5, 130.3, 119.2, 53.4, 42.8, 41.5, 39.4, 19.5, 15.3; HRMS (ESI): *m/z* calcd for C₁₁H₁₉N₄O₂⁺ [M+H]⁺ 239.1503. Found 239.1500.



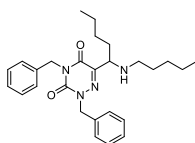
6-(1-(ethylamino)ethyl)-4-methyl-2-(prop-2-yn-1-yl)-1,2,4-triazine-3,5(2H,4H)-dione (**4r**). a yellow liquid (77% yield, 54.8 mg). (PET/EtOAc = 1:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 4.65 (s, 2H), 3.94 (q, *J* = 6.2 Hz, 1H), 3.61 (s, 3H), 2.57-2.54 (m, 2H), 2.19 (s, 1H), 1.86 (s, 1H), 1.34 (d, *J* = 6.2 Hz, 3H), 1.06 (t, *J* = 6.7 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 154.6, 148.0, 146.4, 76.6, 71.5, 53.3, 41.4, 39.3, 29.7, 19.3, 15.2; HRMS (ESI): *m/z* calcd for C₁₁H₁₇N₄O₂⁺ [M+H]⁺ 237.1346. Found 237.1347.



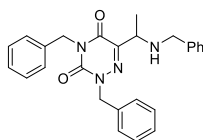
2,4-dibenzyl-6-(1-(propylamino)propyl)-1,2,4-triazine-3,5(2H,4H)-dione (4s). a yellow liquid (67% yield, 79.2 mg). (PET/EtOAc = 1:1 as the eluet). ¹H NMR (400 MHz, CDCl₃) δ: 7.46–7.45 (m, 2H), 7.39–7.37 (m, 2H), 7.34–7.28 (m, 6H), 5.18–5.04 (m, 4H), 3.75 (t, *J* = 6.5 Hz, 1H), 2.39 (t, *J* = 6.6 Hz, 2H), 1.82 (s, 1H), 1.82–1.67 (m, 2H), 1.51–1.35 (m, 2H), 0.89–0.83 (m, 6H); ¹³C NMR (100 MHz, CDCl₃) δ: 155.6, 148.7, 146.1, 135.6, 135.6, 129.2, 128.6, 128.5, 128.1, 127.9, 59.4, 55.2, 49.3, 44.0, 26.4, 23.3, 11.6, 10.4; HRMS (ESI): *m/z* calcd for C₂₃H₂₉N₄O₂⁺ [M+H]⁺ 393.2285. Found 393.2286.



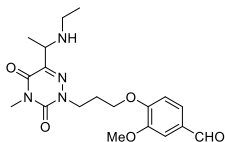
2,4-dibenzyl-6-(1-(butylamino)butyl)-1,2,4-triazine-3,5(2H,4H)-dione (4t). a yellow liquid (63% yield, 78.8 mg). (PET/EtOAc = 1:1 as the eluet). ¹H NMR (400 MHz, CDCl₃) δ: 7.46–7.44 (m, 2H), 7.38–7.28 (m, 8H), 5.18–5.04 (m, 4H), 3.80 (t, *J* = 6.6 Hz, 1H), 2.42 (t, *J* = 7.0 Hz, 2H), 1.82 (s, 1H), 1.77–1.60 (m, 2H), 1.46–1.36 (m, 2H), 1.34–1.22 (m, 4H), 0.91–0.84 (m, 6H); ¹³C NMR (100 MHz, CDCl₃) δ: 155.6, 148.7, 146.4, 135.6, 135.6, 129.2, 128.6, 128.5, 128.1, 127.9, 58.2, 55.1, 47.1, 44.0, 35.7, 32.3, 20.3, 19.3, 13.9, 13.8; HRMS (ESI): *m/z* calcd for C₂₅H₃₃N₄O₂⁺ [M+H]⁺ 421.2598. Found 421.2596.



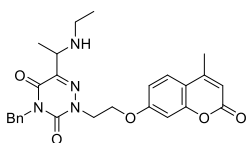
2,4-dibenzyl-6-(1-(pentylamino)pentyl)-1,2,4-triazine-3,5(2H,4H)-dione (4u). a yellow liquid (38% yield, 50.7 mg). (PET/EtOAc = 1:1 as the eluet). ¹H NMR (400 MHz, CDCl₃) δ: 7.45–7.43 (m, 2H), 7.38–7.29 (m, 8H), 5.17–5.04 (m, 4H), 3.79 (t, *J* = 6.6 Hz, 1H), 2.45–2.39 (m, 2H), 1.76 (s, 1H), 1.71–1.65 (m, 4H), 1.29–1.19 (m, 8H), 0.88–0.83 (m, 6H); ¹³C NMR (100 MHz, CDCl₃) δ: 155.6, 148.7, 146.2, 135.7, 135.6, 129.2, 128.7, 128.6, 128.2, 128.0, 58.5, 58.4, 55.2, 47.5, 44.0, 33.3, 29.8, 29.4, 28.3, 22.5, 14.0, 14.0; HRMS (ESI): *m/z* calcd for C₂₇H₃₇N₄O₂⁺ [M+H]⁺ 449.2911. Found 449.2904.



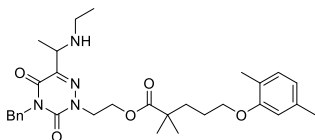
2,4-dibenzyl-6-(1-(benzylamino)ethyl)-1,2,4-triazine-3,5(2H,4H)-dione (4v). a yellow liquid (30% yield, 38.7 mg). (PET/EtOAc = 1:1 as the eluet). ¹H NMR (400 MHz, CDCl₃) δ: 7.49–7.47 (m, 2H), 7.42–7.40 (m, 2H), 7.36–7.31 (m, 6H), 7.17–7.15 (m, 5H), 5.13–5.02 (m, 2H), 4.00 (q, *J* = 6.4 Hz, 1H), 3.67 (q, *J* = 13.2 Hz, 2H), 2.03 (s, 1H), 1.39 (q, *J* = 6.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ: 155.3, 148.7, 146.8, 140.0, 135.6, 135.5, 129.4, 128.7, 128.7, 128.5, 128.5, 128.2, 128.0, 126.8, 126.8, 55.2, 53.6, 51.5, 44.0, 19.7; HRMS (ESI): *m/z* calcd for C₂₆H₂₇N₄O₂⁺ [M+H]⁺ 427.2129. Found 427.2130.



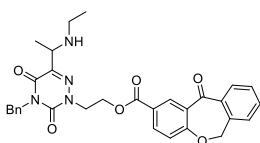
4-(3-(6-(1-(ethylamino)ethyl)-4-methyl-3,5-dioxo-4,5-dihydro-1,2,4-triazin-2(3H)-yl)propoxy)-3-methoxybenzaldehyde (**4w**). a yellow liquid (47% yield, 36.7 mg). (PET/EtOAc = 1:1 as the eluent). ^1H NMR (400 MHz, CDCl_3) δ : 9.81 (s, 1H), 7.40 (d, $J = 7.9$ Hz, 1H), 7.35 (s, 1H), 6.90 (d, $J = 8.1$ Hz, 1H), 4.16 (t, $J = 6.0$ Hz, 4H), 3.92 (q, $J = 6.5$ Hz, 1H), 3.84 (s, 3H), 3.57 (s, 3H), 2.58–2.54 (m, 2H), 2.37 (s, 1H), 2.28–2.22 (m, 2H), 1.31 (d, $J = 6.7$ Hz, 3H), 1.06 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 190.9, 155.8, 153.6, 149.6, 148.9, 145.8, 130.0, 126.8, 111.3, 109.0, 67.2, 55.8, 53.4, 41.4, 39.4, 38.6, 19.2, 15.1; HRMS (ESI): m/z calcd for $\text{C}_{19}\text{H}_{27}\text{N}_4\text{O}_5^+$ $[\text{M}+\text{H}]^+$ 391.1976. Found 391.1975.



4-benzyl-6-(1-(ethylamino)ethyl)-2-(2-((4-methyl-2-oxo-2H-chromen-7-yl)oxy)ethyl)-1,2,4-triazine-3,5-dione (**4x**). a yellow liquid (33% yield, 47.1 mg). (PET/EtOAc = 1:1 as the eluent). ^1H NMR (400 MHz, CDCl_3) δ : 7.45–7.43 (m, 1H), 7.40–7.38 (m, 2H), 7.34–7.32 (m, 2H), 7.24 (s, 1H), 6.78–6.76 (m, 2H), 6.12 (s, 1H), 5.19–5.04 (m, 2H), 4.39–4.36 (m, 2H), 4.27 (d, $J = 5.5$ Hz, 2H), 4.05 (q, $J = 6.8$ Hz, 1H), 2.66–2.52 (m, 2H), 2.37 (s, 3H), 1.40 (d, $J = 6.6$ Hz, 3H), 1.10 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 161.1, 161.1, 155.5, 155.1, 152.4, 148.5, 145.3, 135.3, 130.4, 128.7, 128.5, 128.3, 125.6, 113.9, 112.2, 101.7, 64.1, 55.4, 53.1, 41.2, 39.4, 18.9, 18.6, 14.6; HRMS (ESI): m/z calcd for $\text{C}_{26}\text{H}_{29}\text{N}_4\text{O}_5^+$ $[\text{M}+\text{H}]^+$ 477.2132. Found 477.2125.

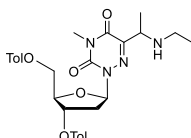


2-(4-benzyl-6-(1-(ethylamino)ethyl)-3,5-dioxo-4,5-dihydro-1,2,4-triazin-2(3H)-yl)ethyl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (**4y**). a yellow liquid (62% yield, 102.3 mg). (PET/EtOAc = 1:1 as the eluent). ^1H NMR (400 MHz, CDCl_3) δ : 7.39–7.37 (m, 2H), 7.35–7.30 (m, 3H), 6.99 (d, $J = 7.3$ Hz, 1H), 6.65 (d, $J = 7.4$ Hz, 1H), 6.60 (s, 1H), 5.17–5.02 (m, 2H), 4.35–4.29 (m, 2H), 4.23–4.21 (m, 2H), 3.96 (q, $J = 6.6$ Hz, 1H), 3.89–3.86 (m, 2H), 2.52 (q, $J = 7.0$ Hz, 2H), 2.30 (s, 3H), 2.17 (s, 3H), 2.01 (s, 1H), 1.70–1.63 (m, 4H), 1.36 (d, $J = 6.7$ Hz, 3H), 1.12 (s, 6H), 1.07 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 177.4, 156.8, 155.4, 148.5, 146.5, 136.3, 135.5, 130.2, 128.6, 128.6, 128.1, 123.4, 120.6, 111.8, 67.8, 60.6, 55.1, 53.4, 41.9, 41.4, 39.8, 36.8, 24.9, 24.9, 21.3, 19.6, 15.7, 15.2; HRMS (ESI): m/z calcd for $\text{C}_{31}\text{H}_{43}\text{N}_4\text{O}_5^+$ $[\text{M}+\text{H}]^+$ 551.3228. Found 551.3227.



2-(4-benzyl-6-(1-(ethylamino)ethyl)-3,5-dioxo-4,5-dihydro-1,2,4-triazin-2(3H)-yl)ethyl 11-oxo-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-5-ylideneacetate (**4z**). a yellow liquid (33% yield, 47.1 mg). (PET/EtOAc = 1:1 as the eluent).

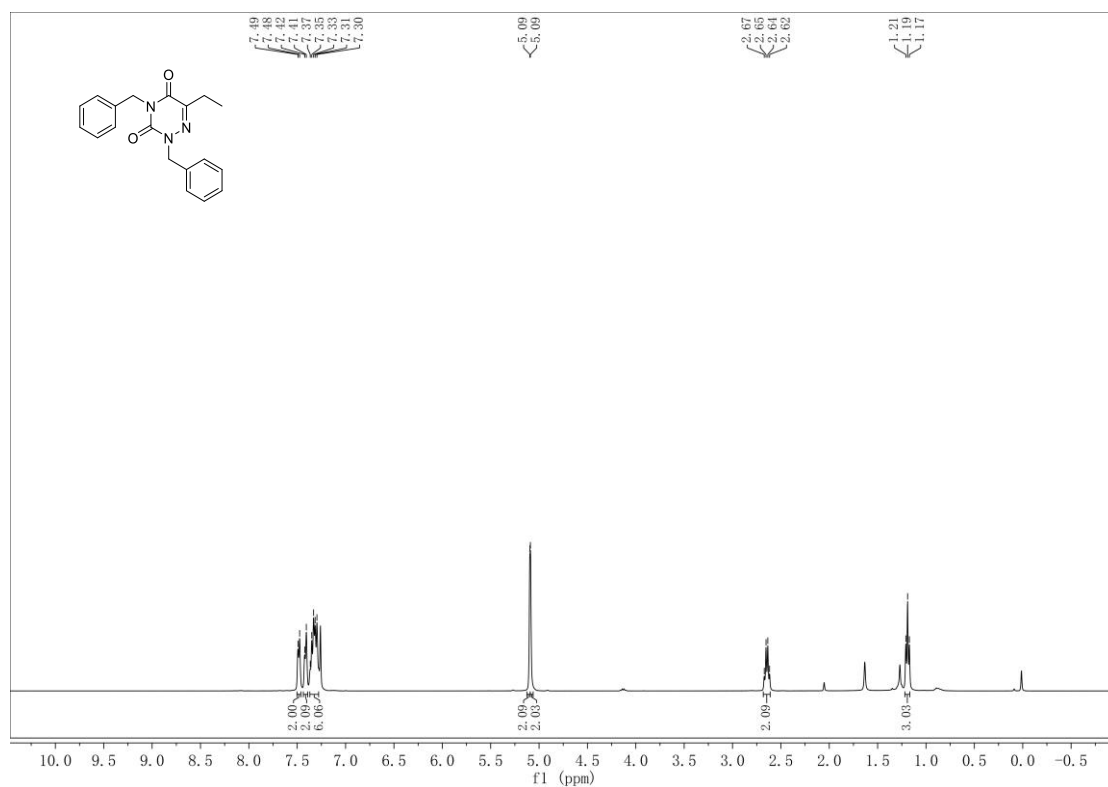
1-dihydrodibenzo[b,e]loxepine-2-carboxylate (4z). a yellow liquid (46% yield, 74.6 mg). (PET/EtOAc = 1:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 8.05–8.04 (m, 1H), 7.88–7.86 (m, 1H), 7.57–7.53 (m, 1H), 7.48–7.44 (m, 1H), 7.40–7.35 (m, 5H), 7.33–7.31 (m, 2H), 7.01 (d, *J* = 8.4 Hz, 1H), 5.18–5.04 (m, 4H), 4.35–4.34 (m, 2H), 4.24–4.20 (m, 2H), 4.04–3.99 (m, 1H), 3.49 (s, 2H), 2.63–2.62 (m, 1H), 2.60–2.55 (m, 2H), 1.41–1.39 (m, 3H), 1.11–1.08 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 190.8, 171.3, 160.4, 155.6, 148.7, 145.8, 140.4, 136.5, 135.5, 135.5, 132.7, 132.5, 129.5, 129.2, 128.3, 127.8, 127.4, 125.0, 121.0, 73.6, 61.2, 55.4, 53.3, 41.4, 39.7, 19.3, 14.9; HRMS (ESI): *m/z* calcd for C₃₁H₃₁N₄O₆⁺ [M+H]⁺ 555.2238. Found 555.2234.



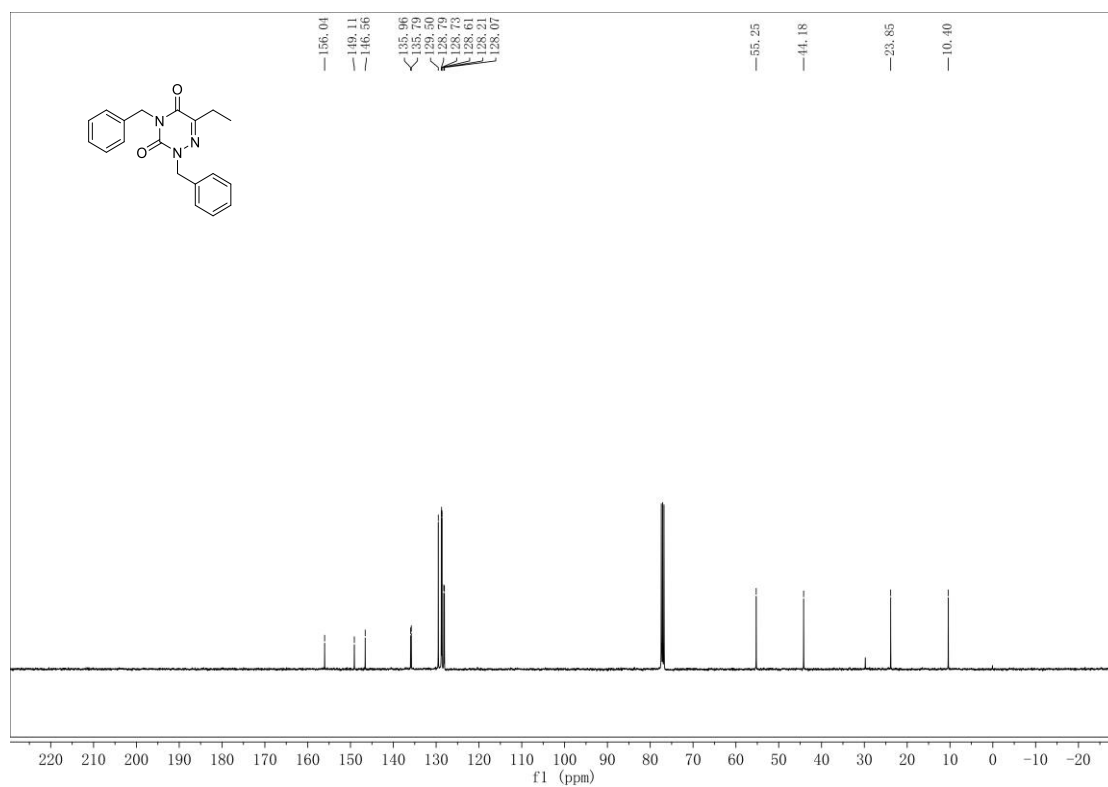
(2R,3S,5R)-5-(6-(1-(ethylamino)ethyl)-4-methyl-3,5-dioxo-4,5-dihydro-1,2,4-triazin-2(3H)-yl)-2-(((4-methylbenzoyl)oxy)methyl)tetrahydrofuran-3-yl 4-methylbenzoate (4aa). a yellow liquid (30% yield, 49.5 mg). (PET/EtOAc = 1:1 as the eluent). ¹H NMR (400 MHz, CDCl₃) δ: 7.94–7.92 (m, 2H), 7.87–7.86 (m, 2H), 7.26–7.25 (m, 2H), 7.20–7.18 (m, 2H), 6.74–6.71 (m, 1H), 5.74–5.71 (m, 1H), 4.57–4.56 (m, 1H), 4.53–4.50 (m, 1H), 3.36 (s, 3H), 3.06–3.01 (m, 1H), 2.59–2.53 (m, 2H), 2.52–2.51 (m, 1H), 2.43 (s, 3H), 2.39 (s, 3H), 1.58 (s, 1H), 1.27–1.25 (m, 3H), 1.24–1.23 (m, 2H), 0.88–0.83 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 192.1, 166.2, 166.0, 152.7, 148.6, 144.5, 144.1, 137.6, 129.8, 129.6, 129.2, 129.2, 126.7, 126.3, 87.4, 82.4, 74.2, 63.7, 35.2, 29.7, 27.8, 27.5, 21.7, 21.7; HRMS (ESI): *m/z* calcd for C₂₉H₃₅N₄O₇⁺ [M+H]⁺ 551.2500. Found 551.2502.

X. NMR charts of 3a-4u

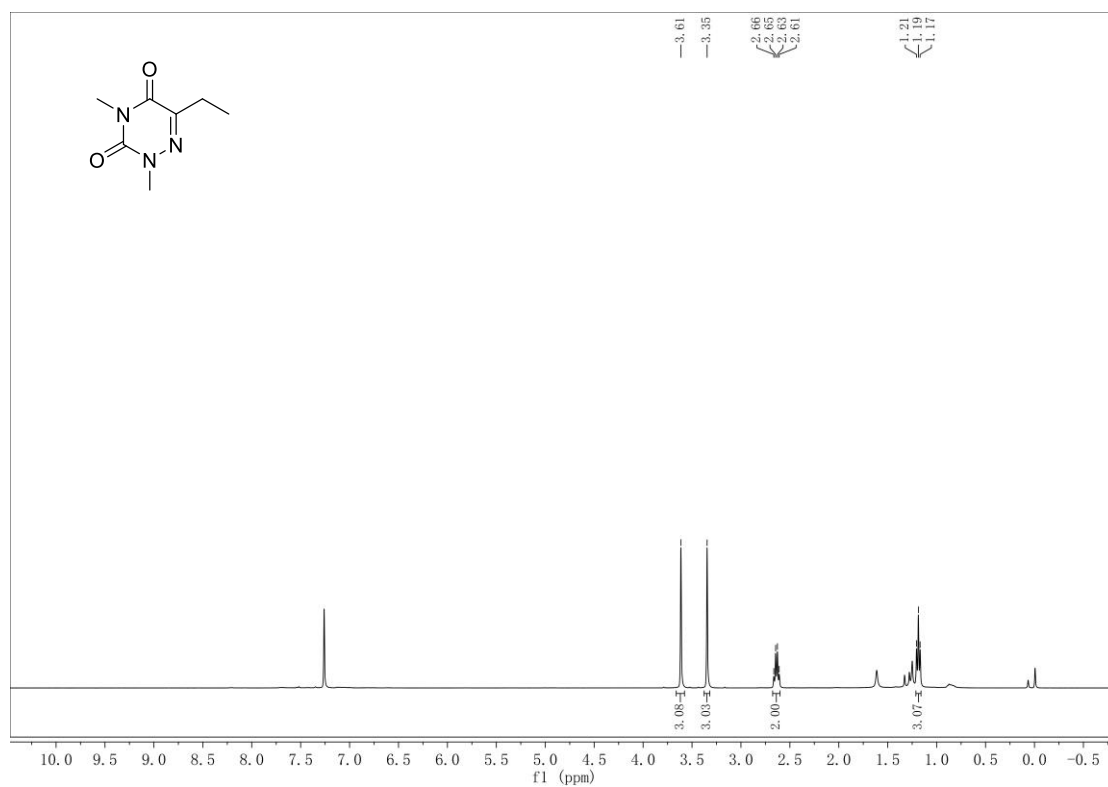
3a-¹H



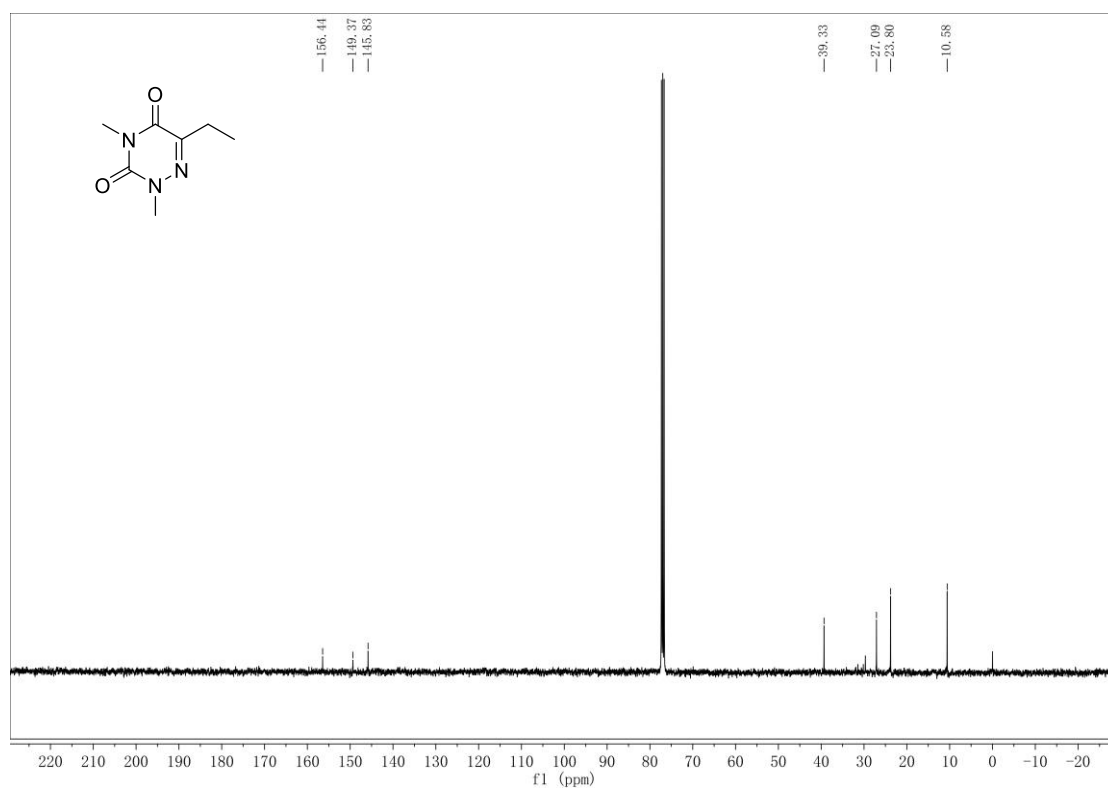
3a-¹³C

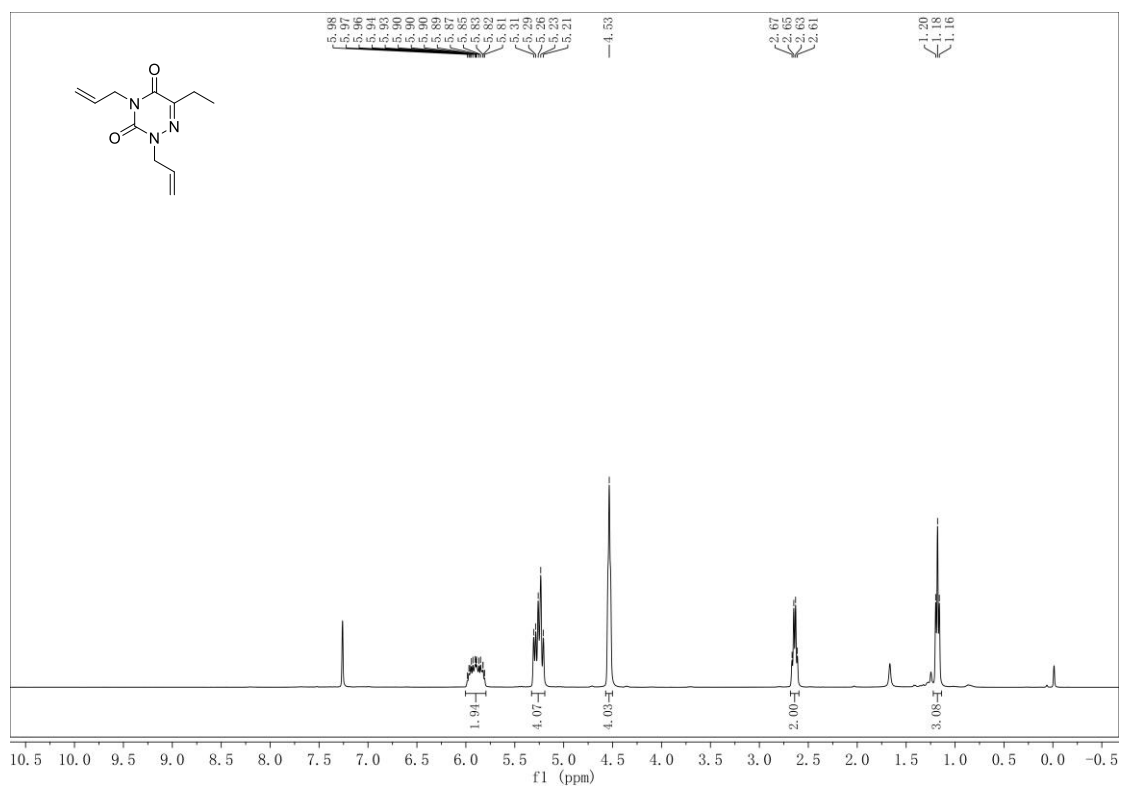
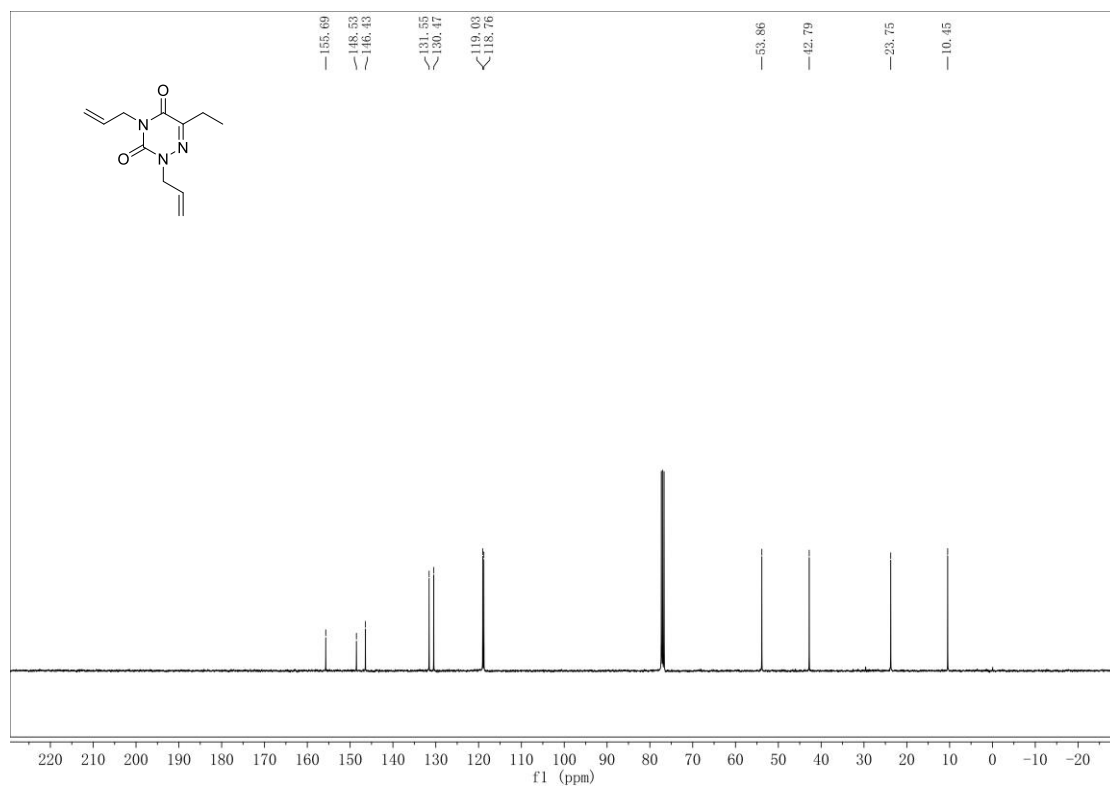


3b-¹H

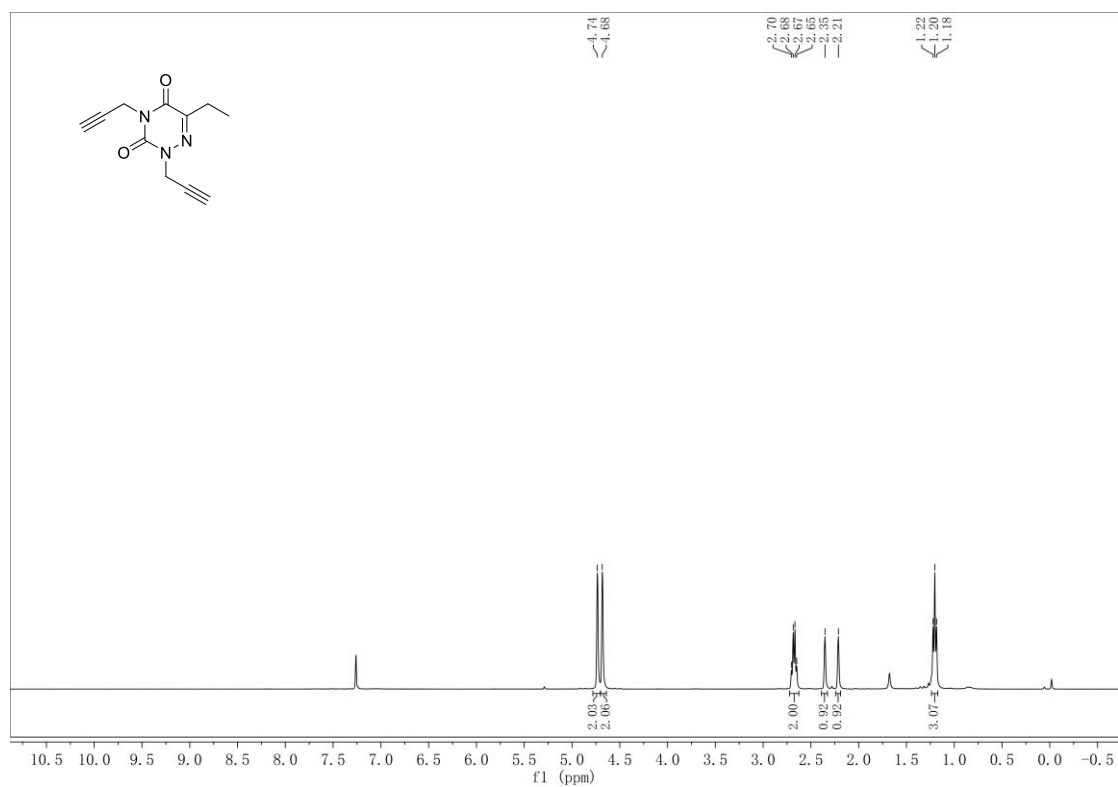


3b-¹³C

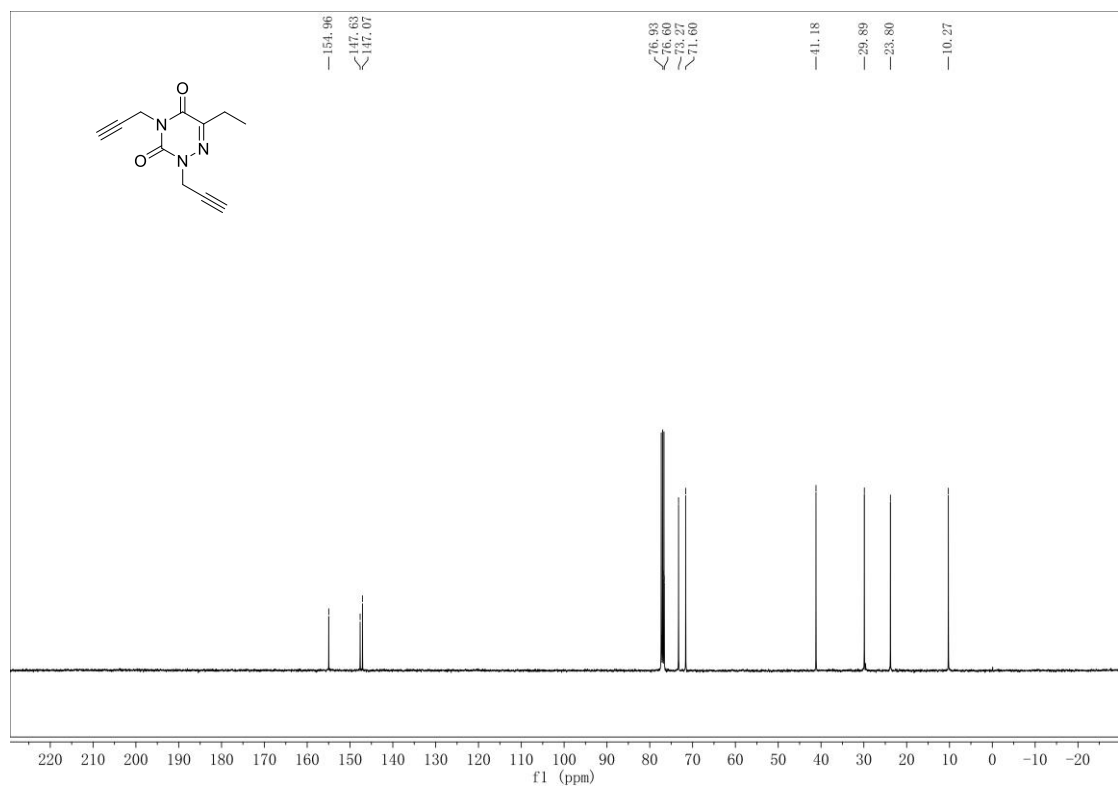


3c-¹H**3c-¹³C**

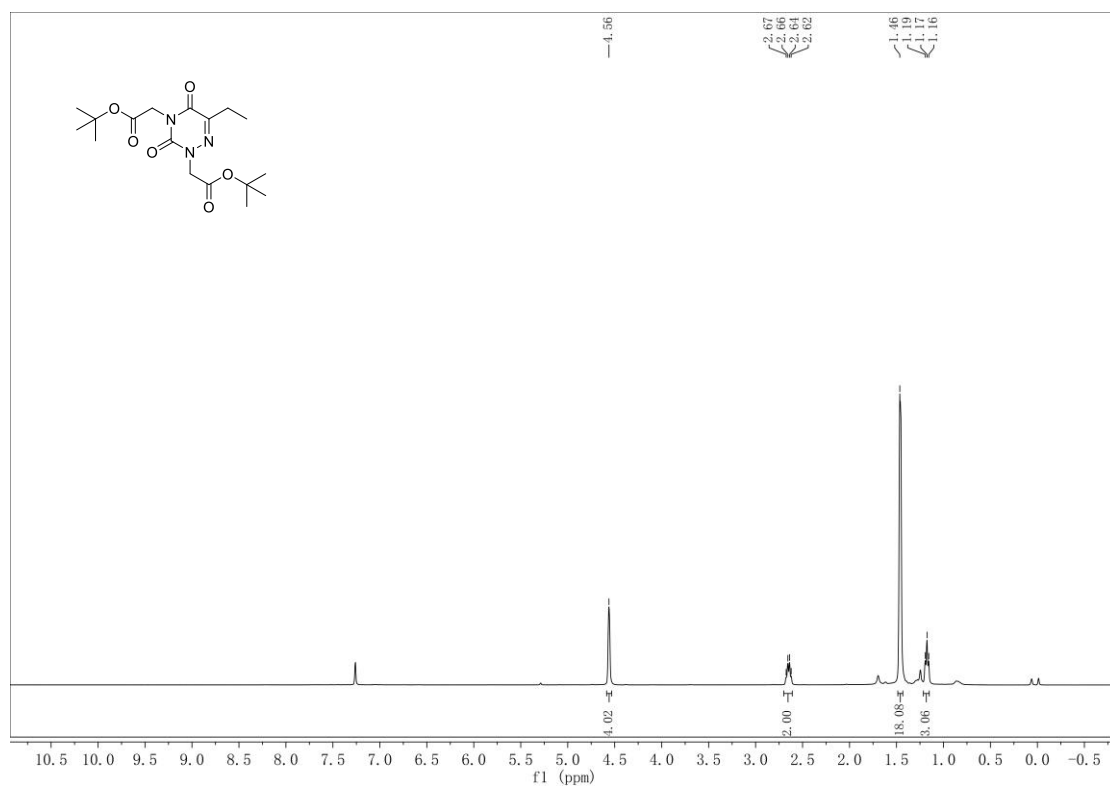
3d-¹H



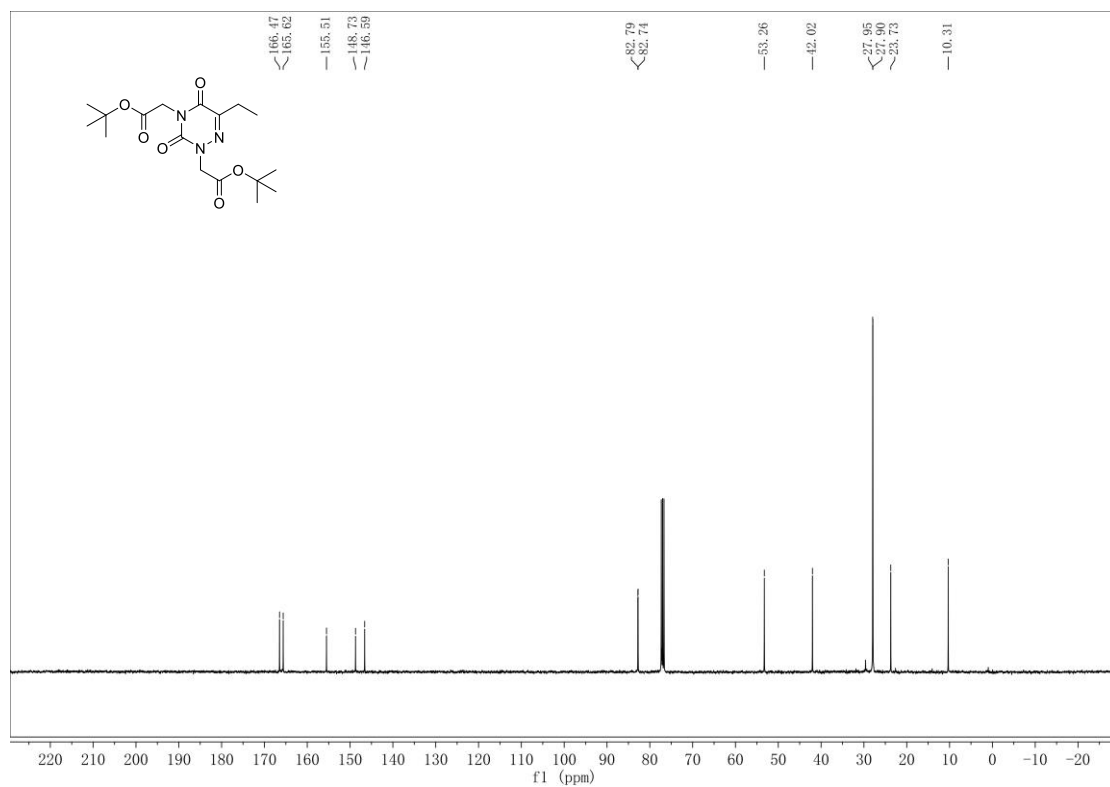
3d-¹³C



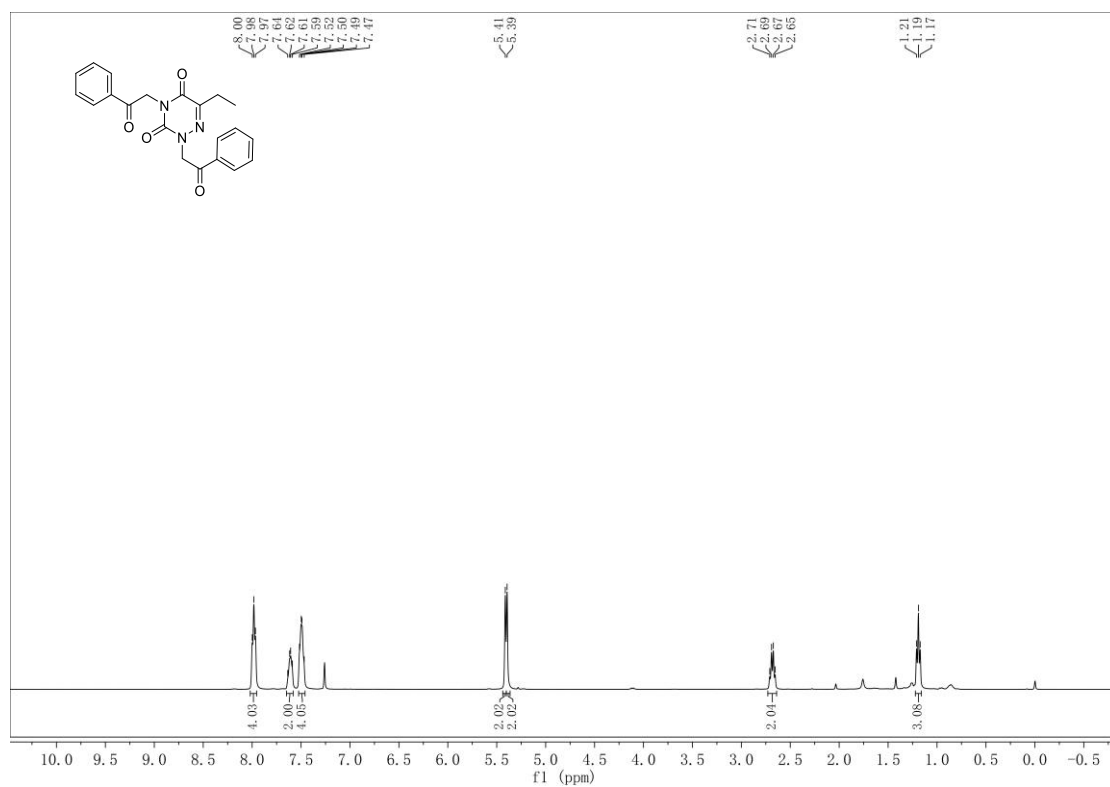
3e-¹H



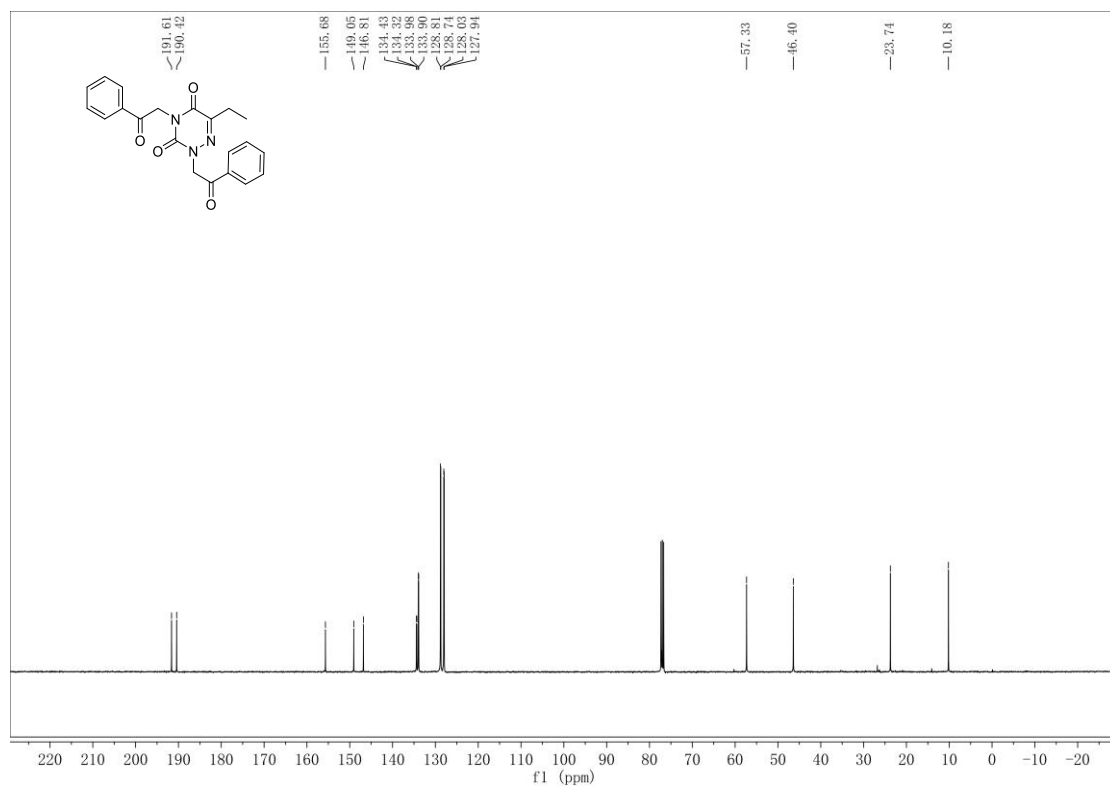
3e-¹³C



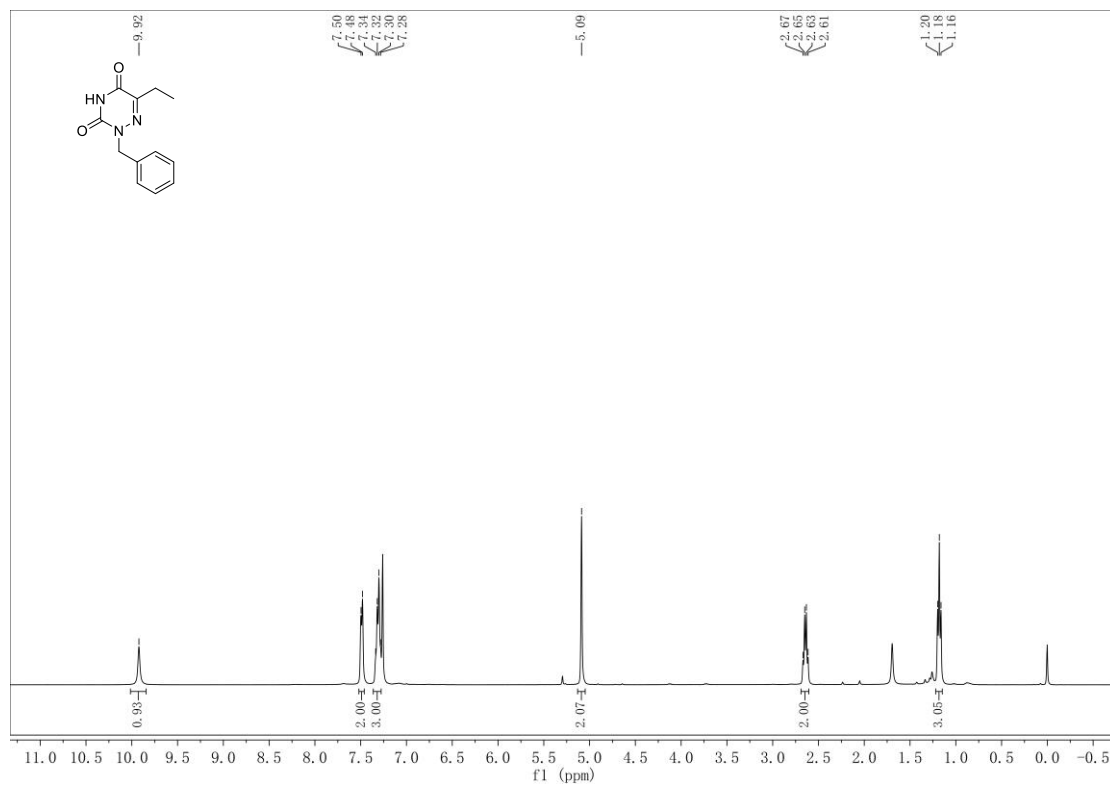
3f-¹H



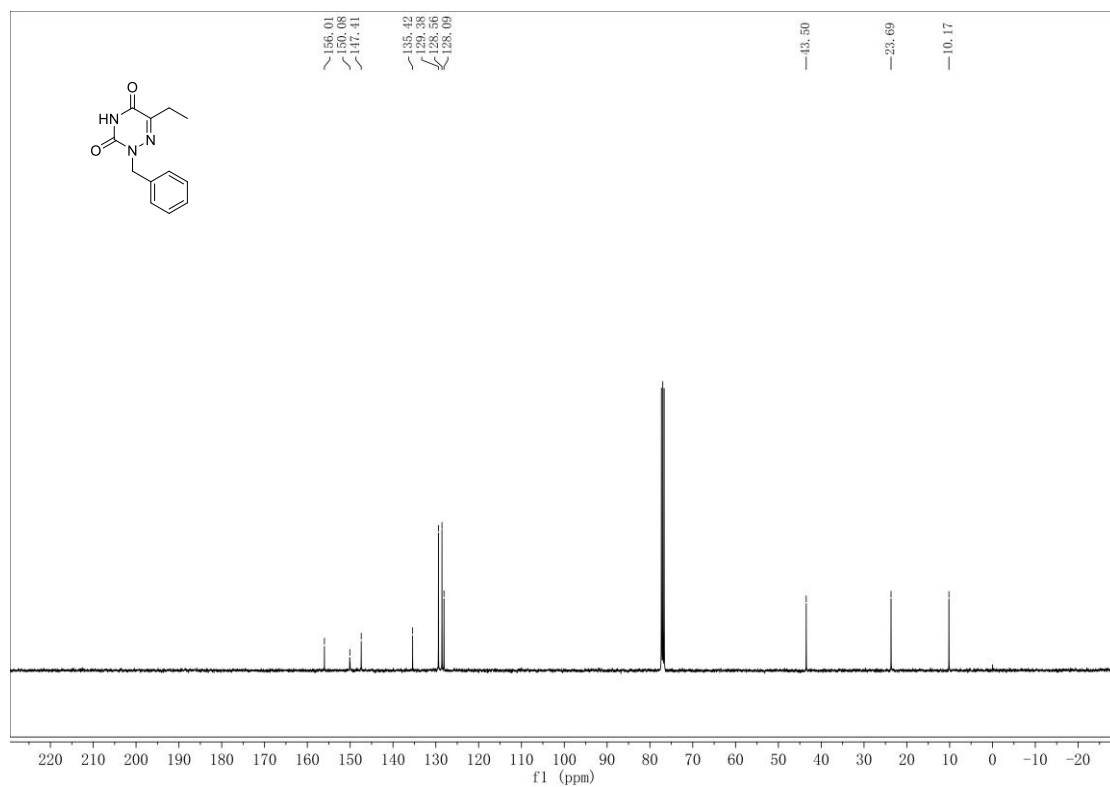
4f-¹³C



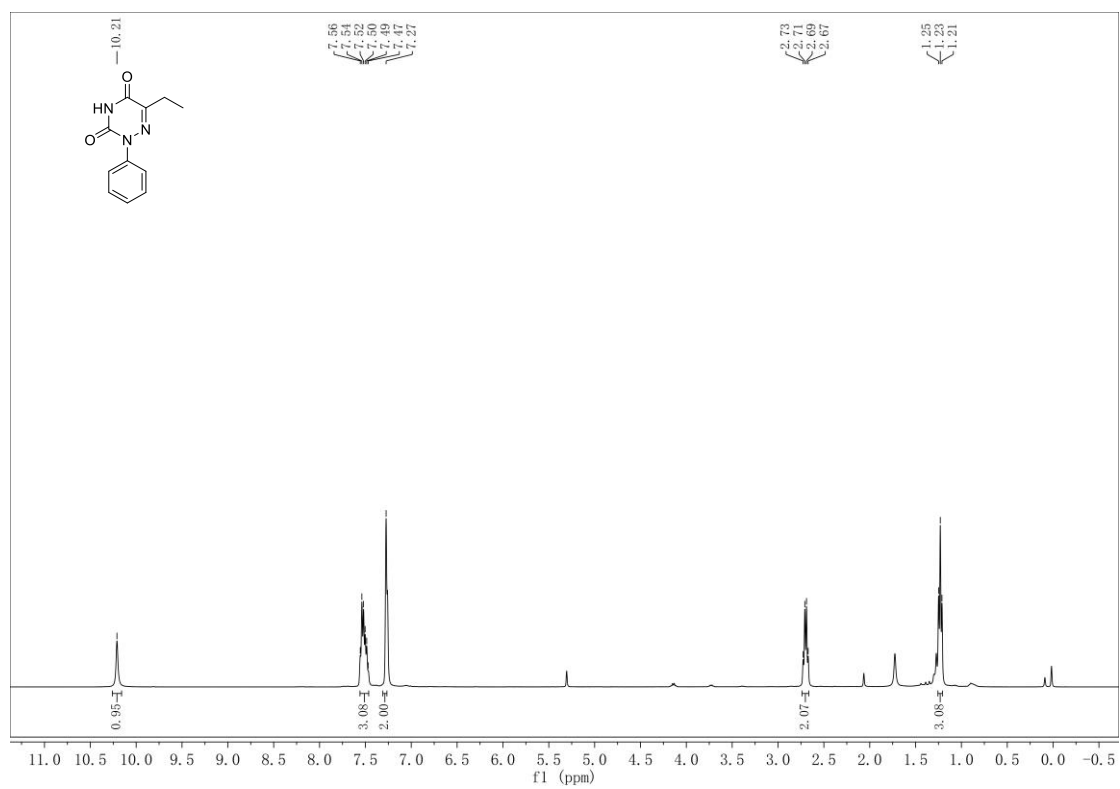
3g-¹H



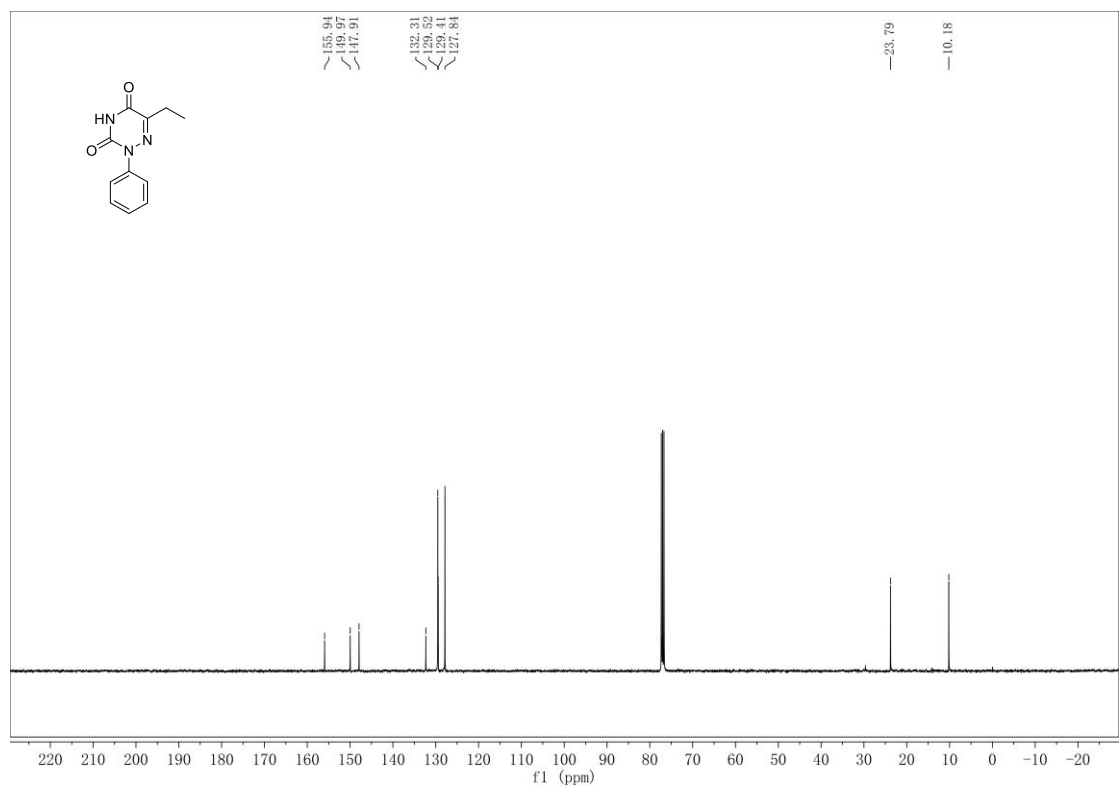
3g-¹³C



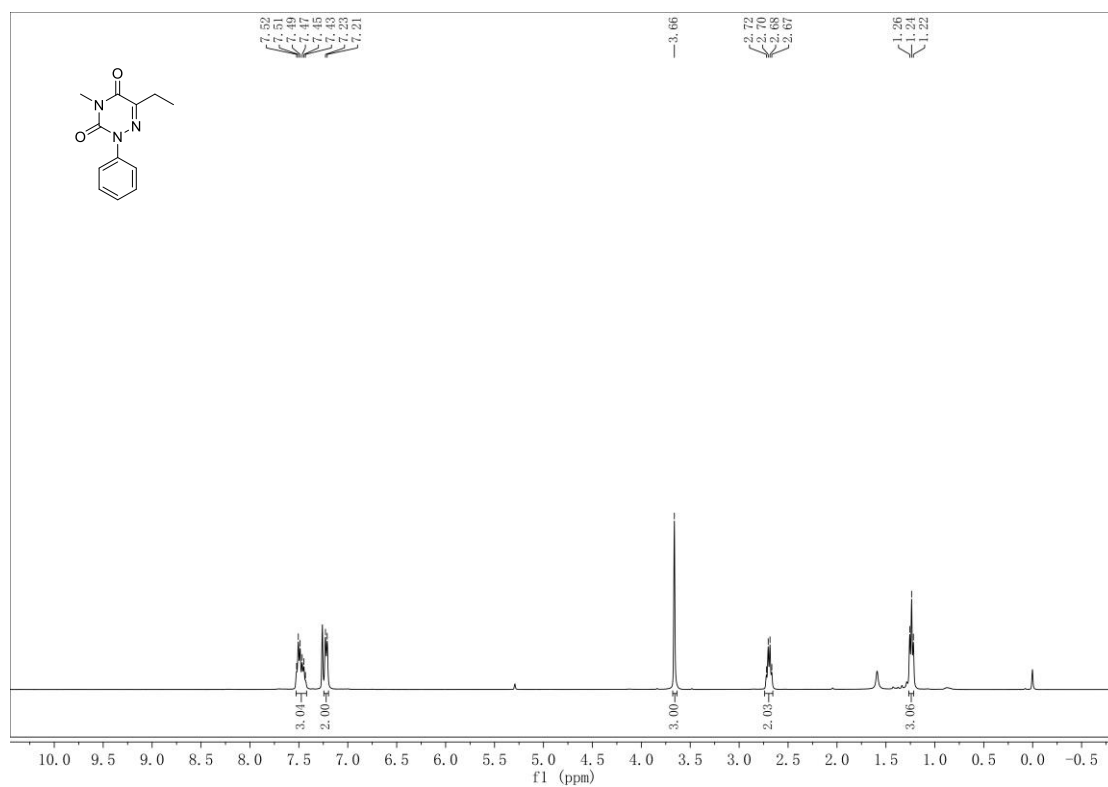
3h-¹H



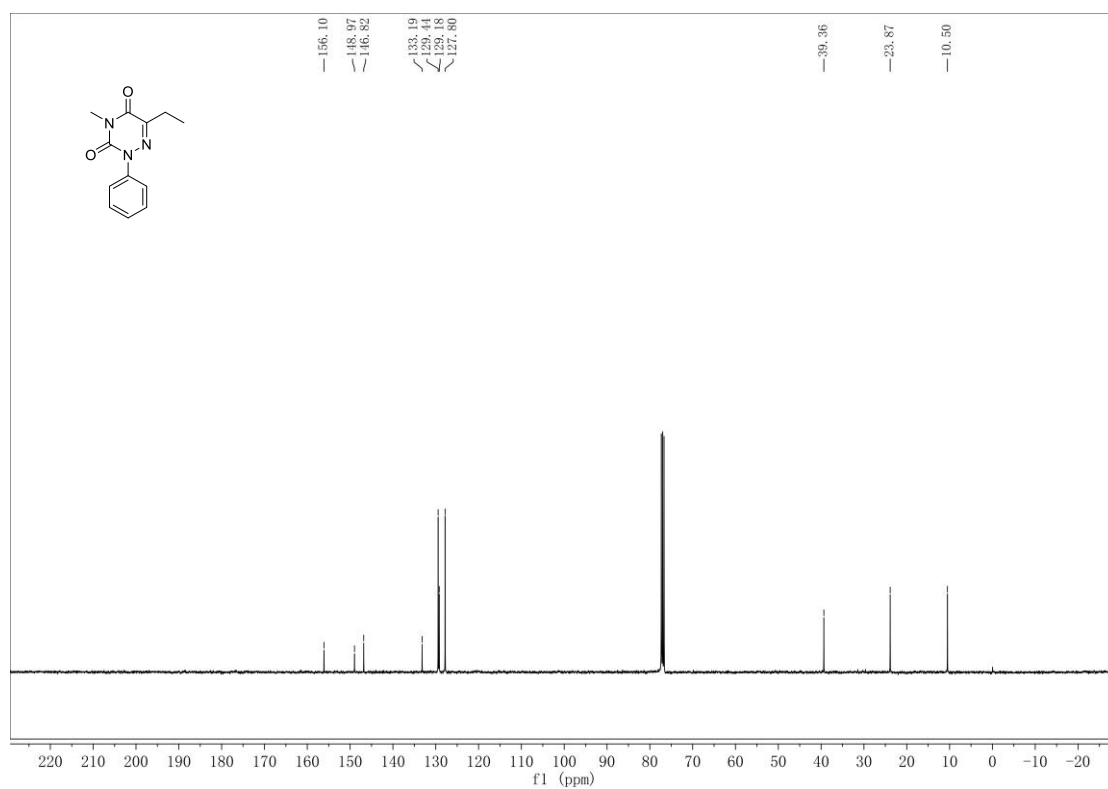
3h-¹³C



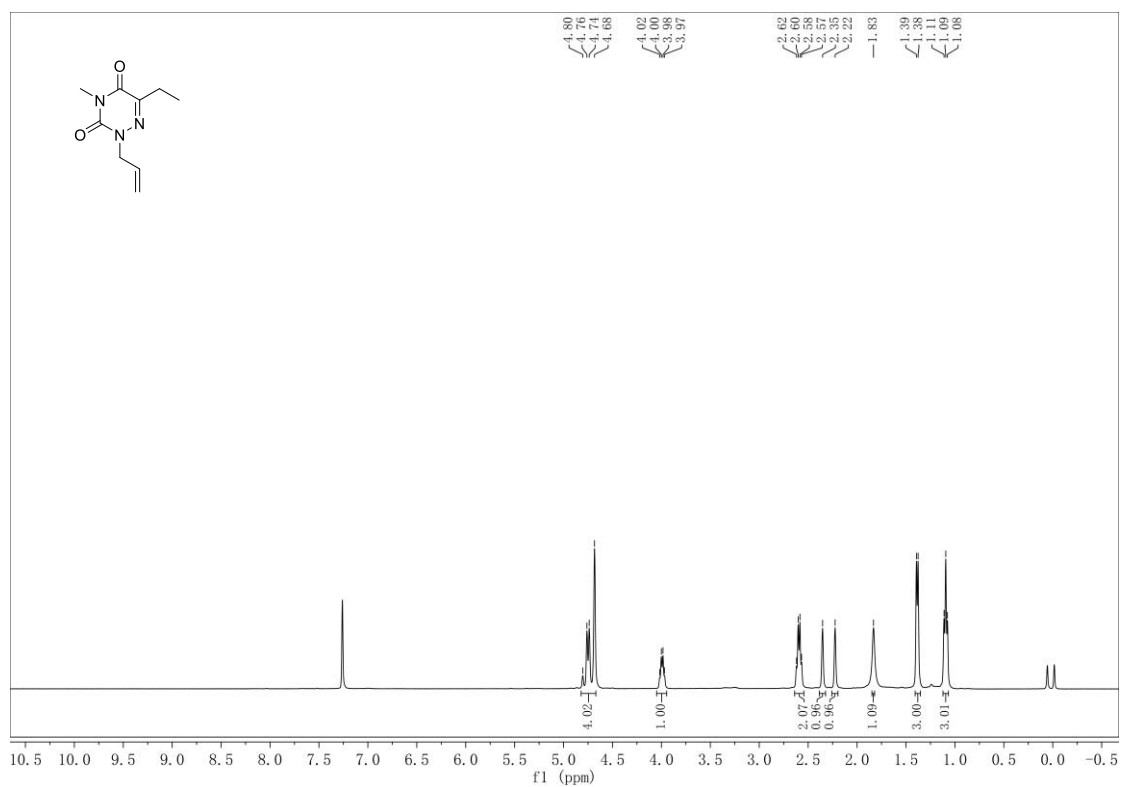
3i-¹H



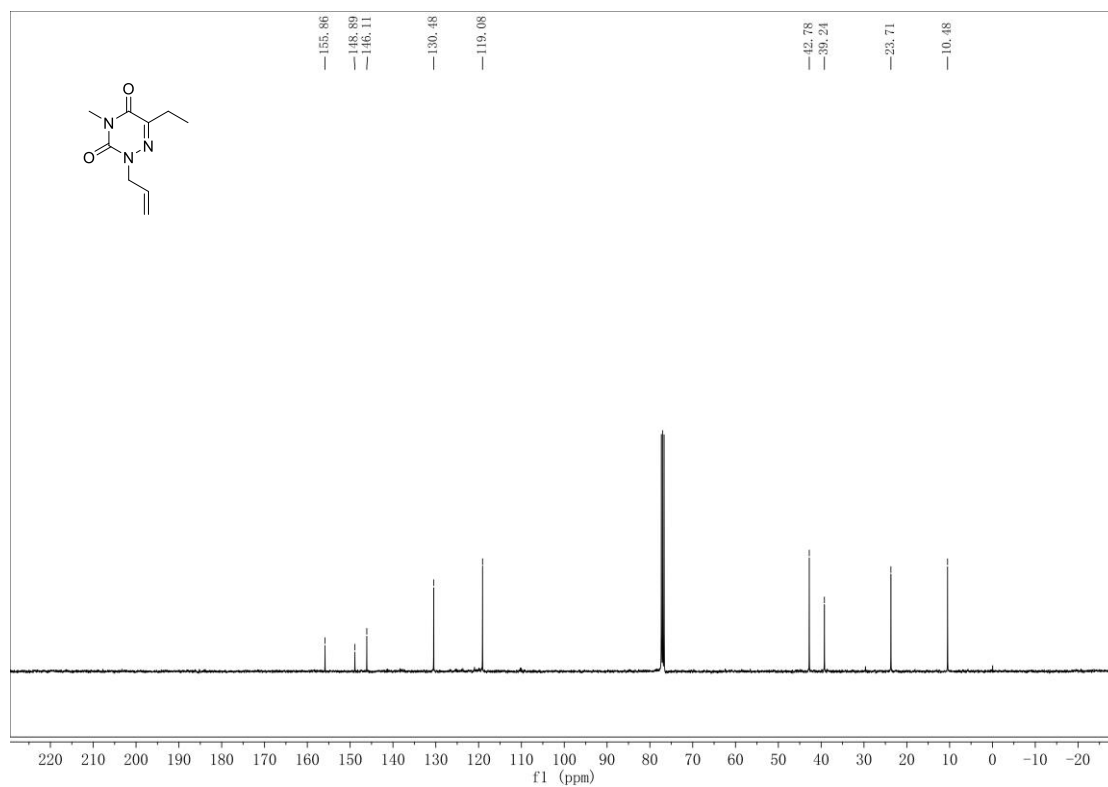
3i-¹³C



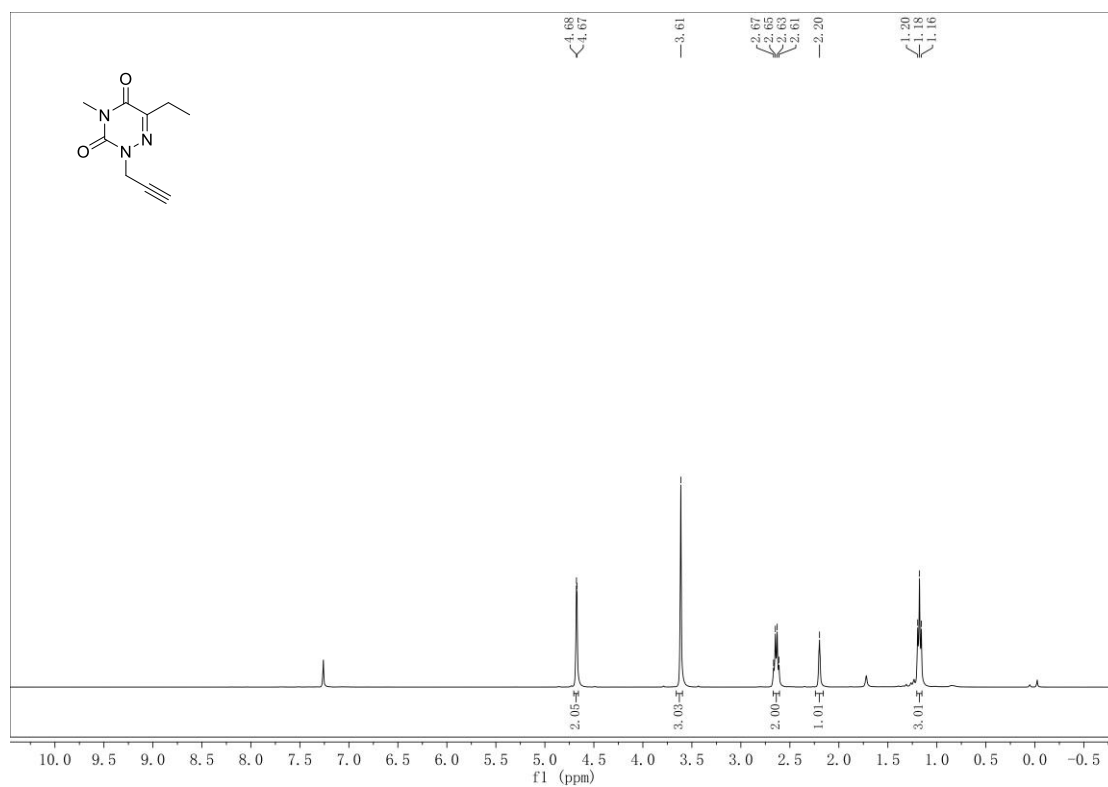
3j-¹H



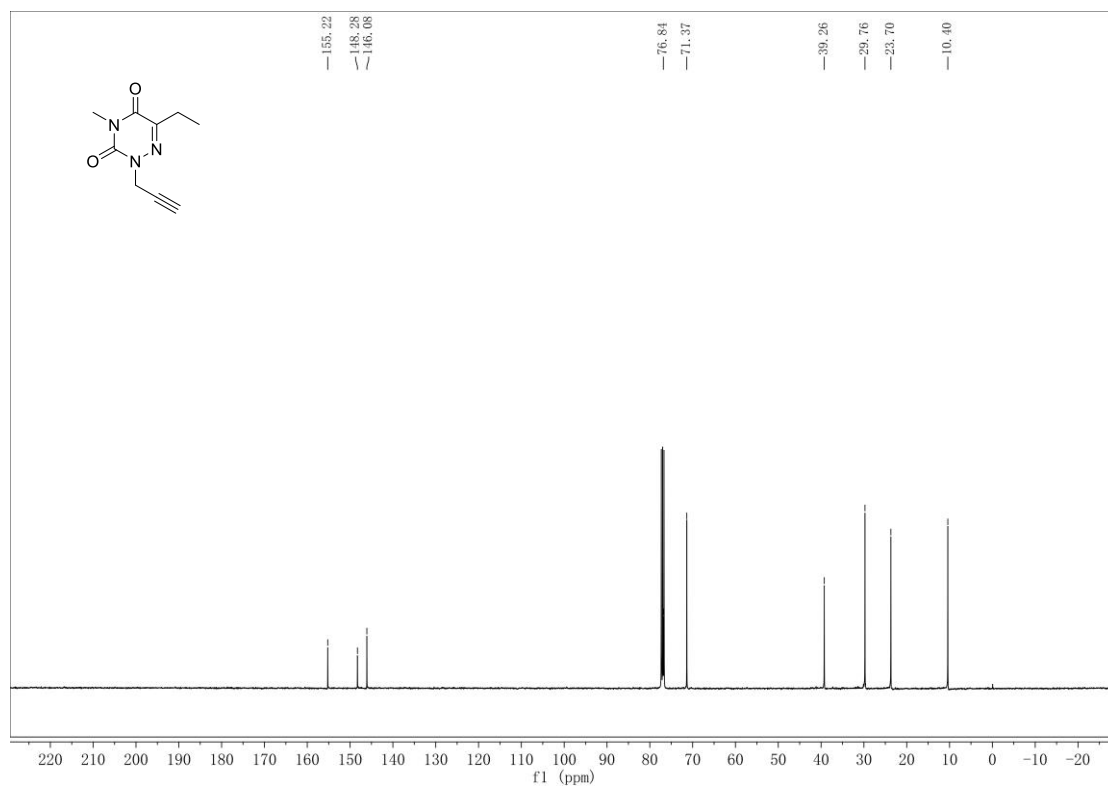
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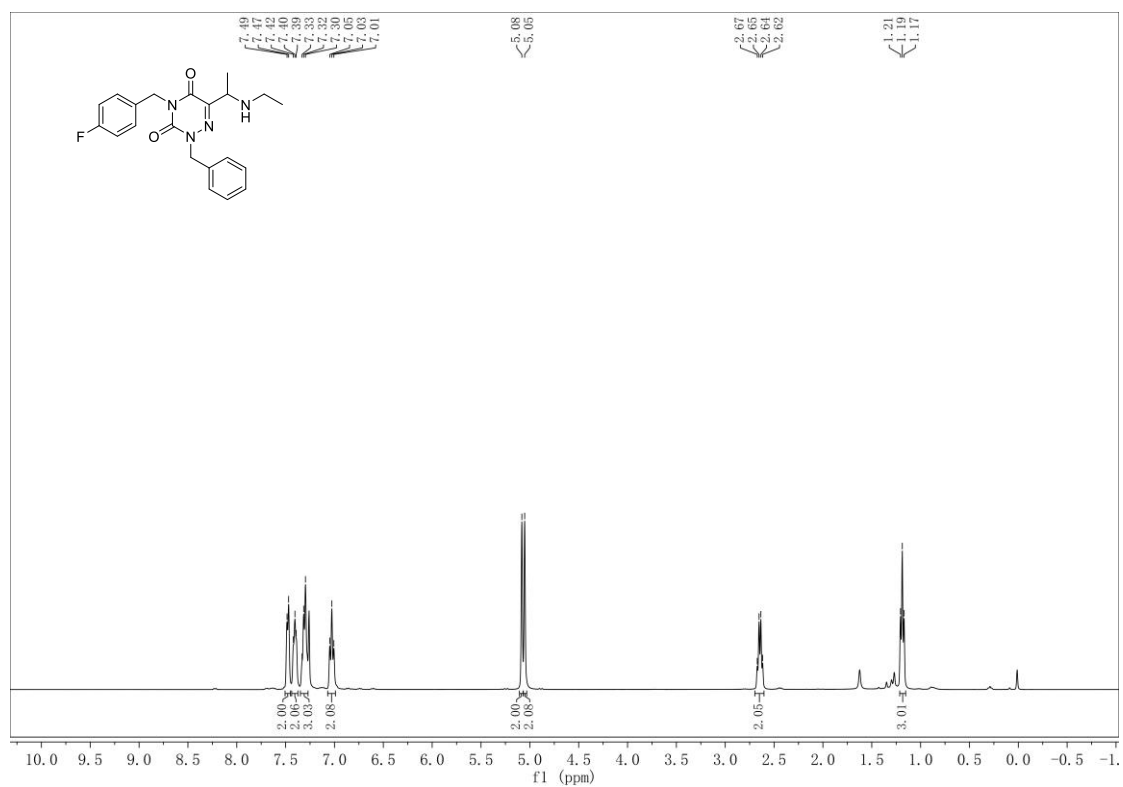
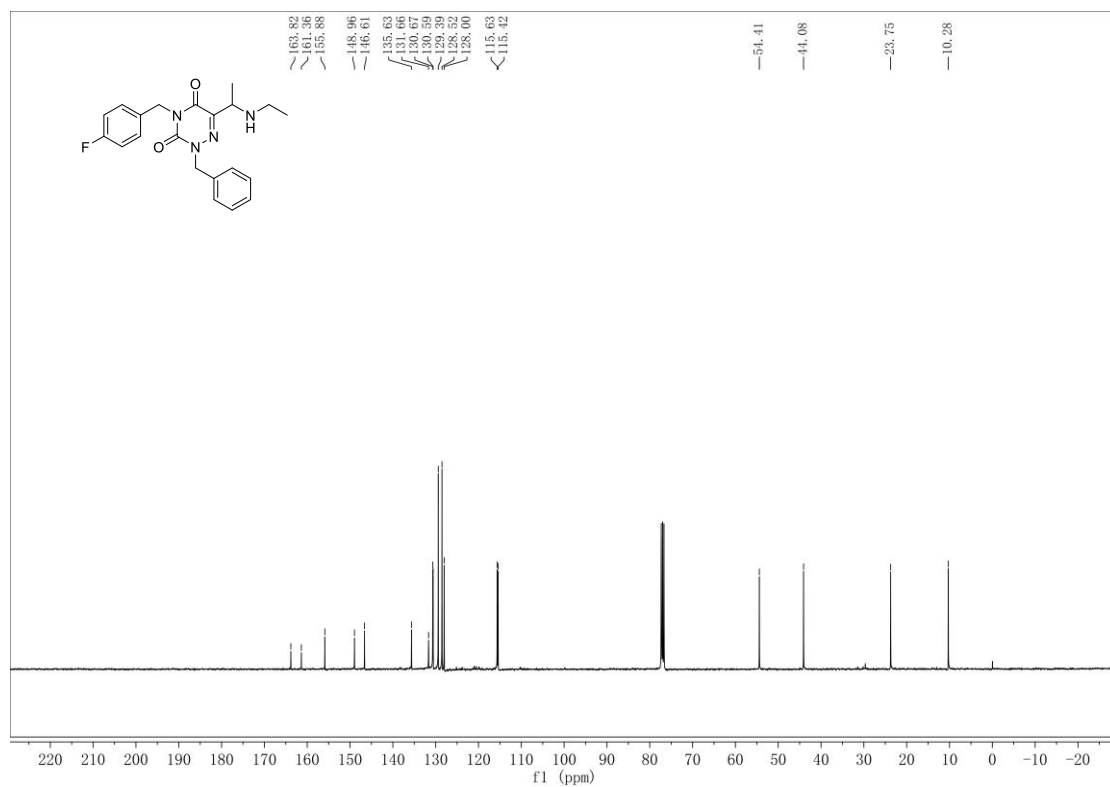


3k-¹H

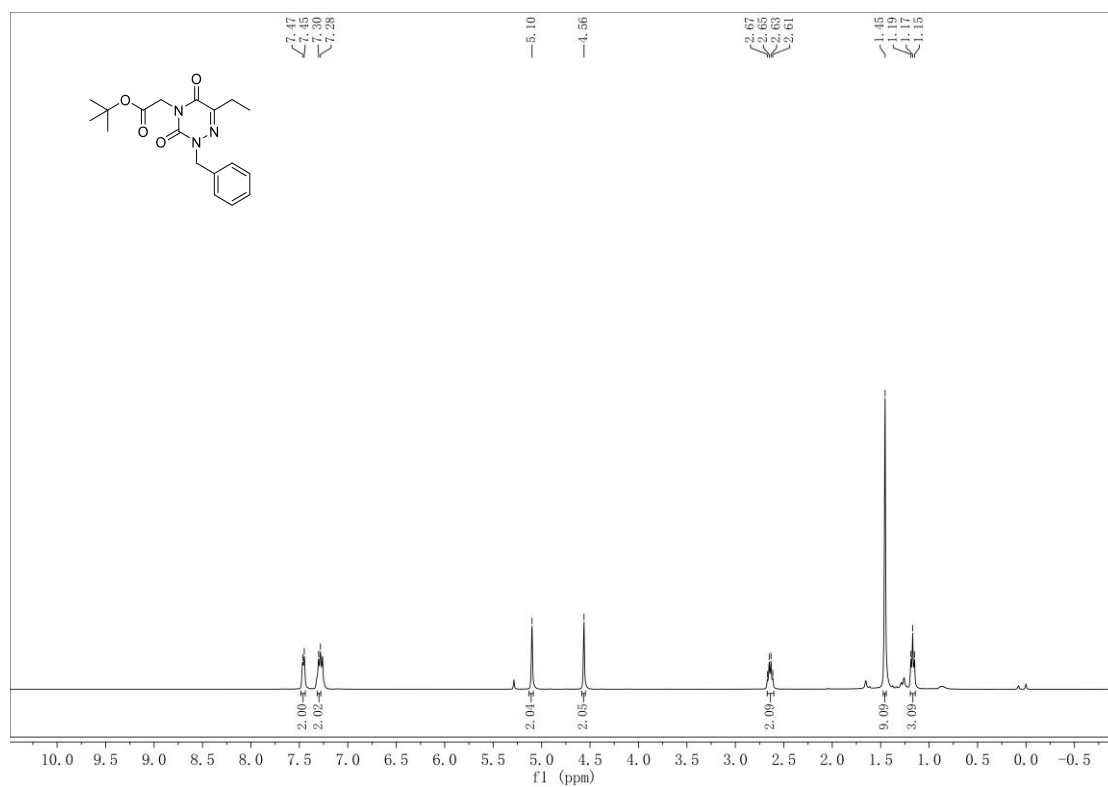


3k-¹³C

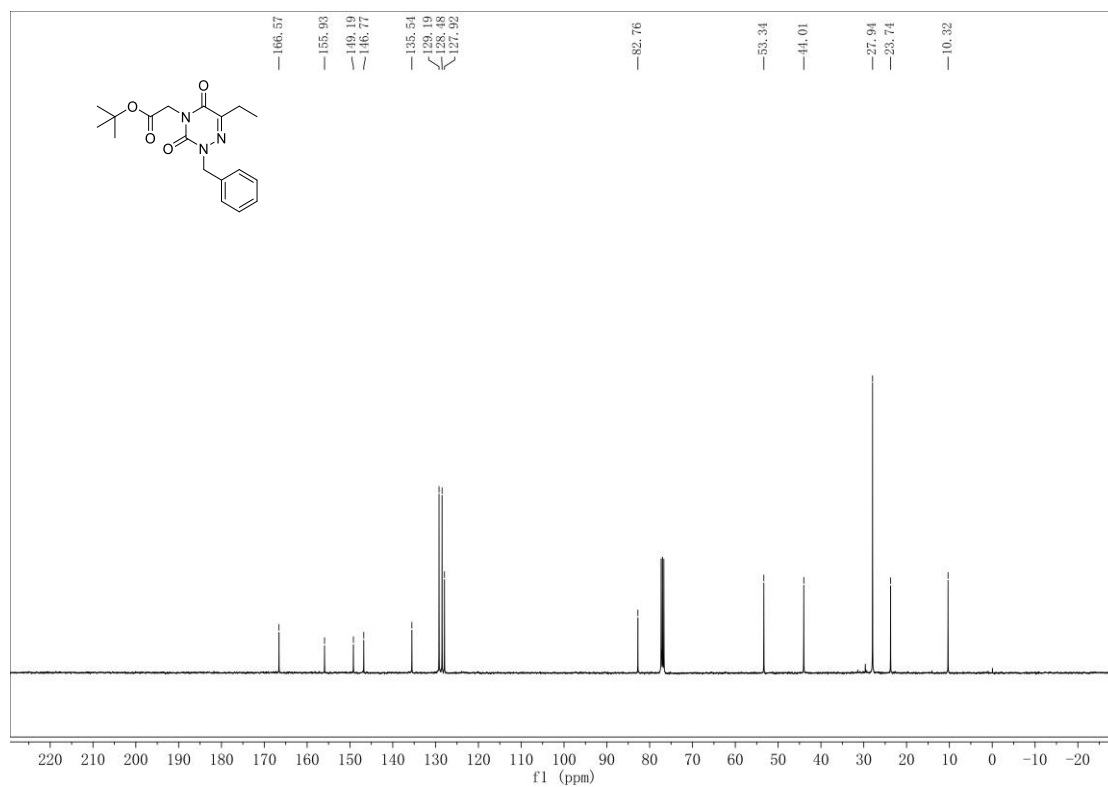


31-¹H**31-¹³C**

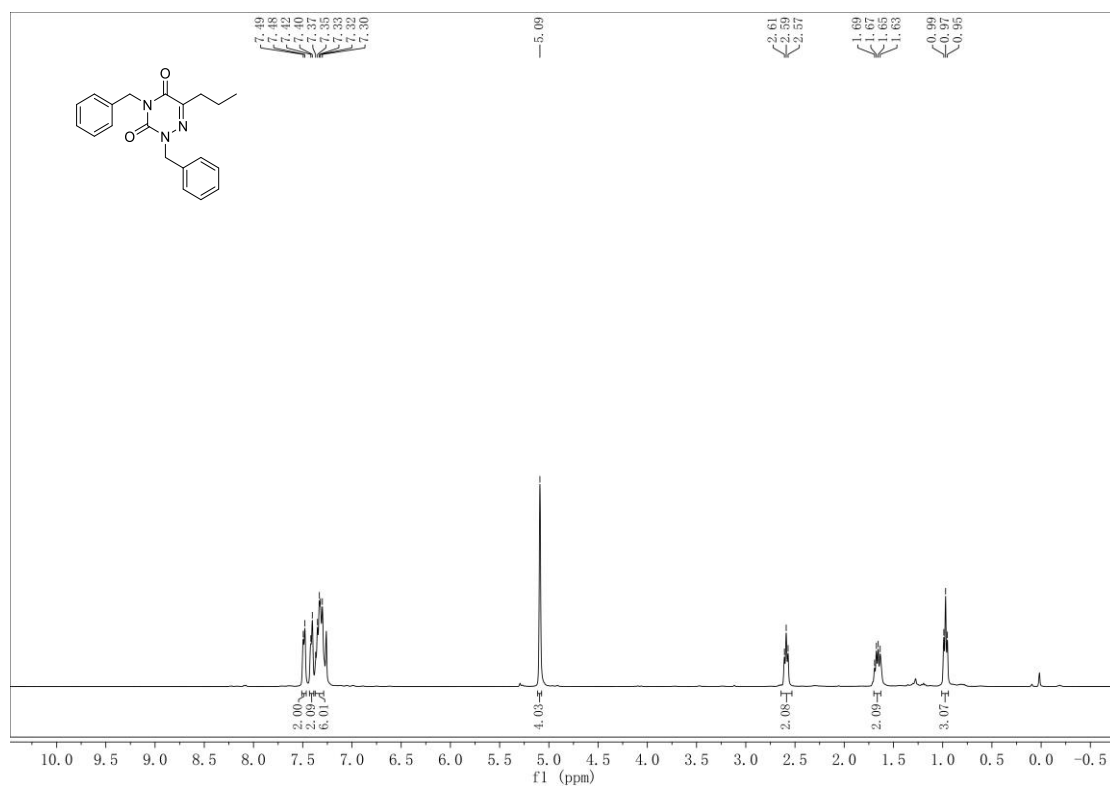
3m-¹H



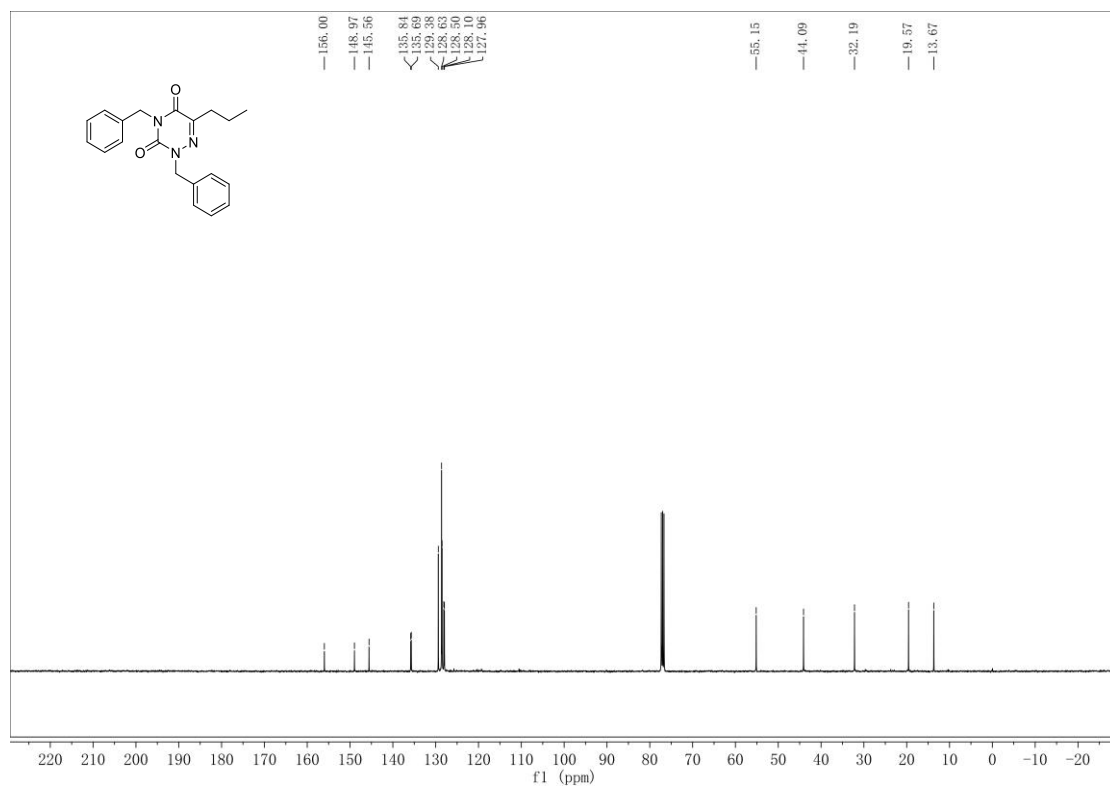
3m-¹³C



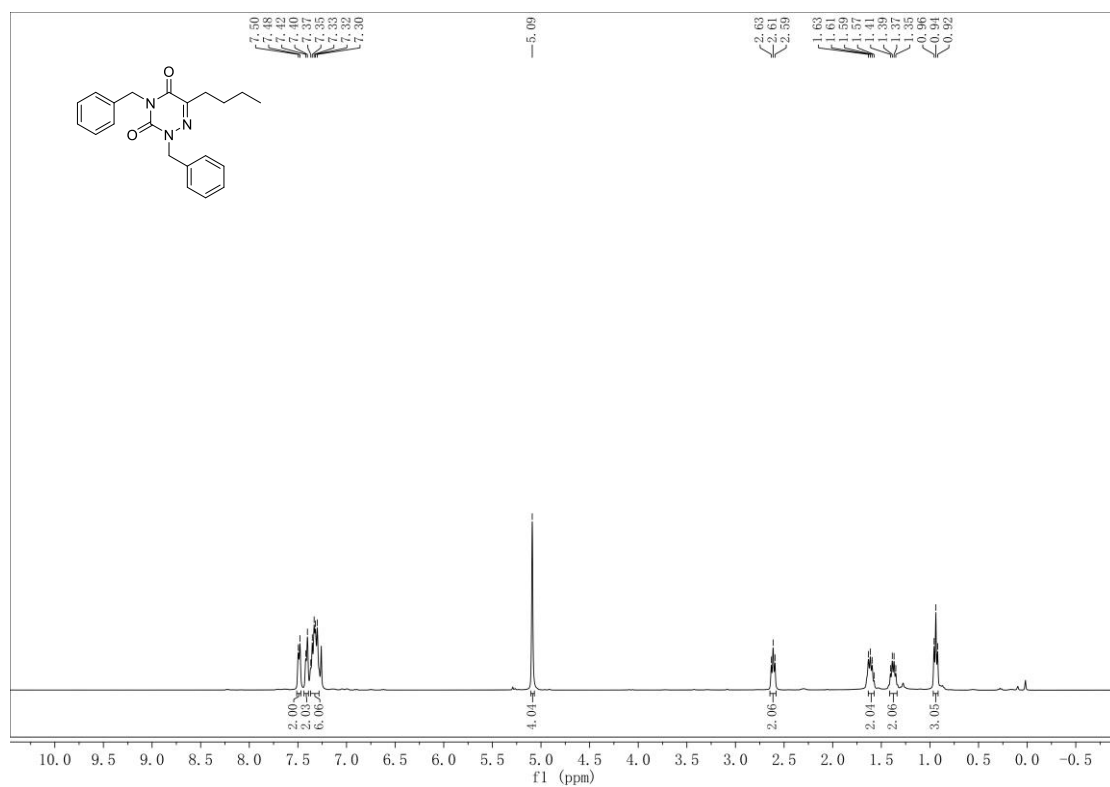
3n-¹H



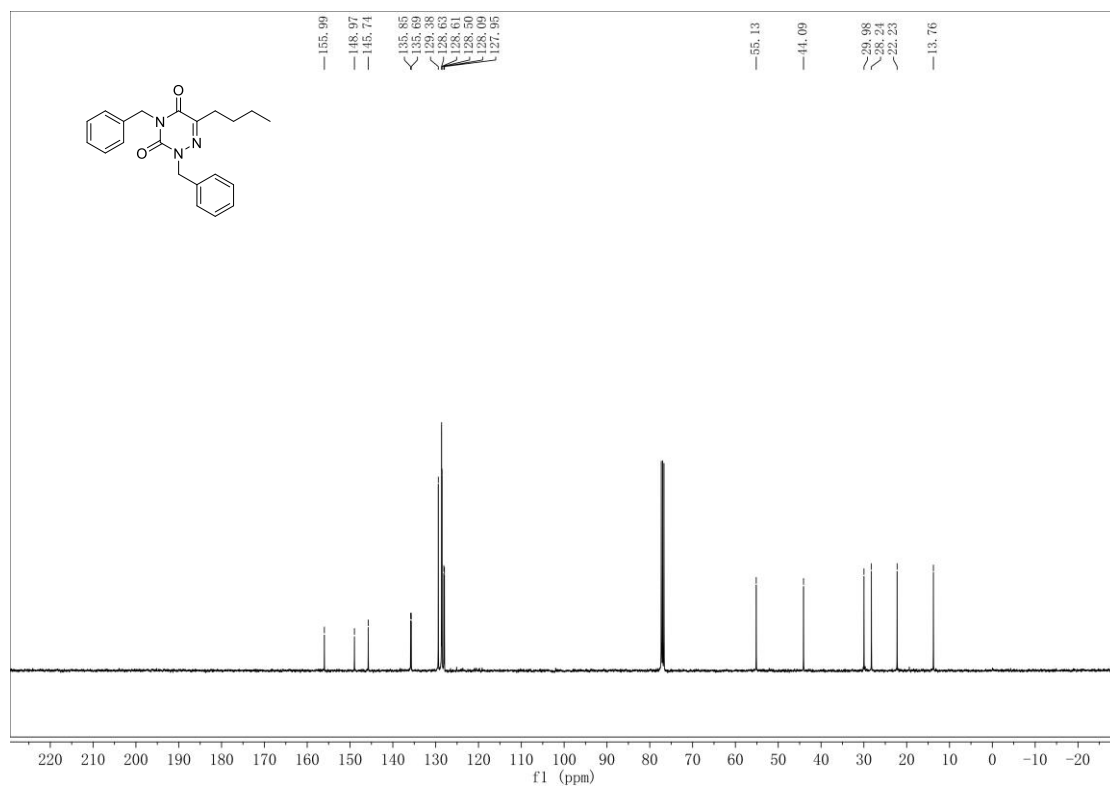
3n-¹³C



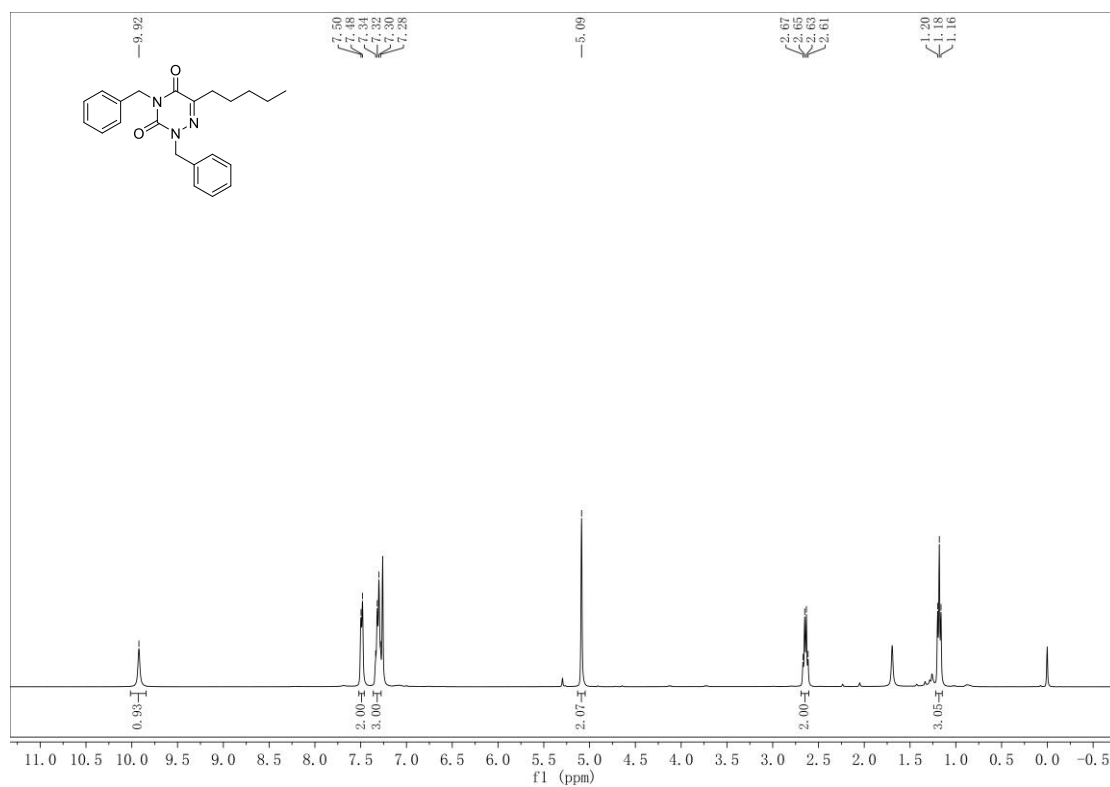
30-¹H



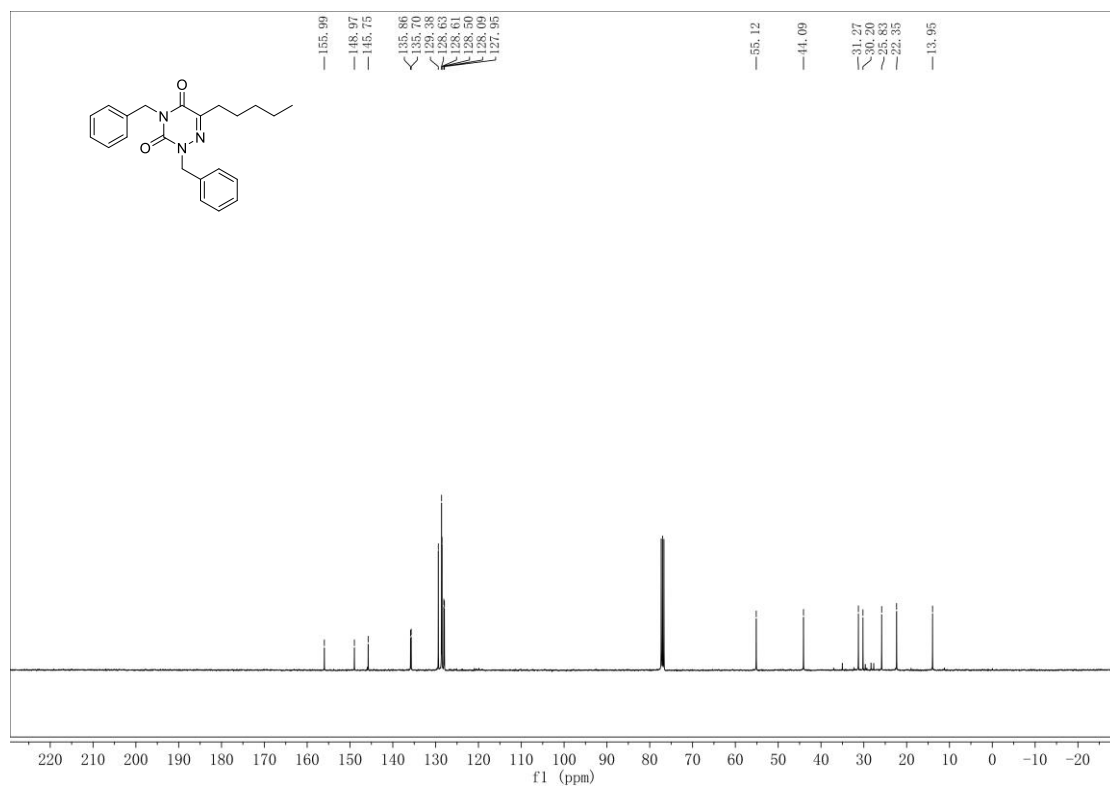
30-¹³C



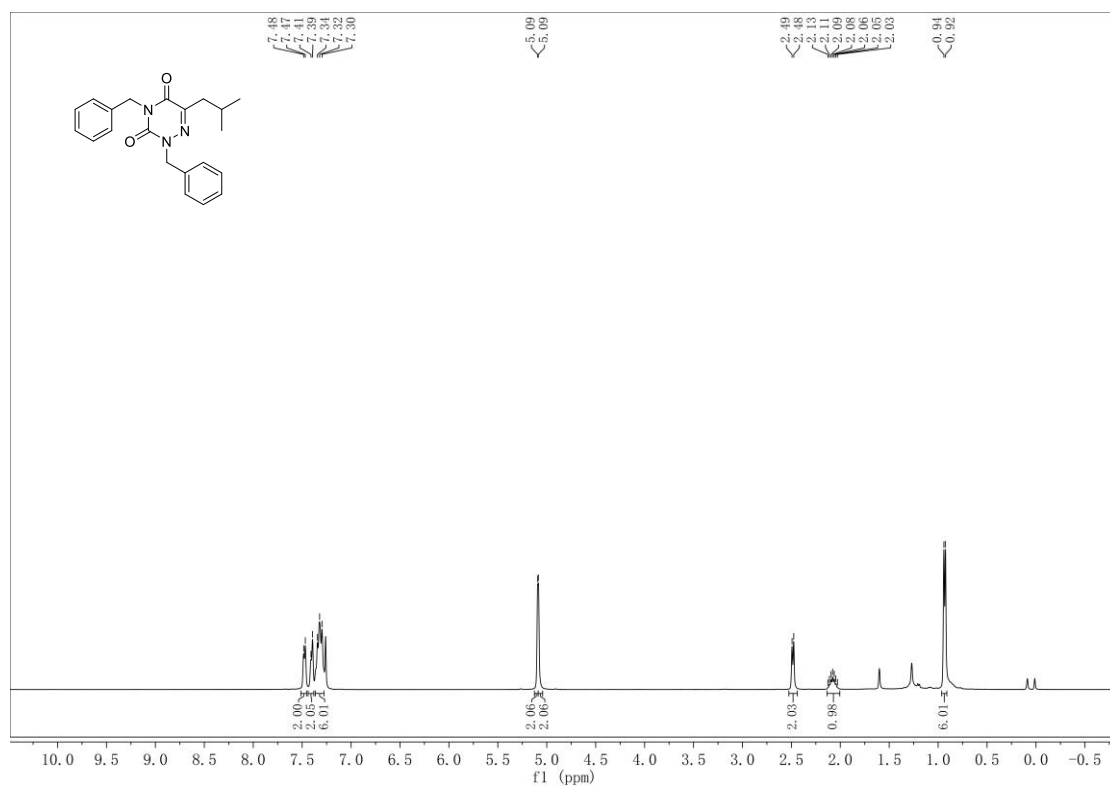
3p-¹H



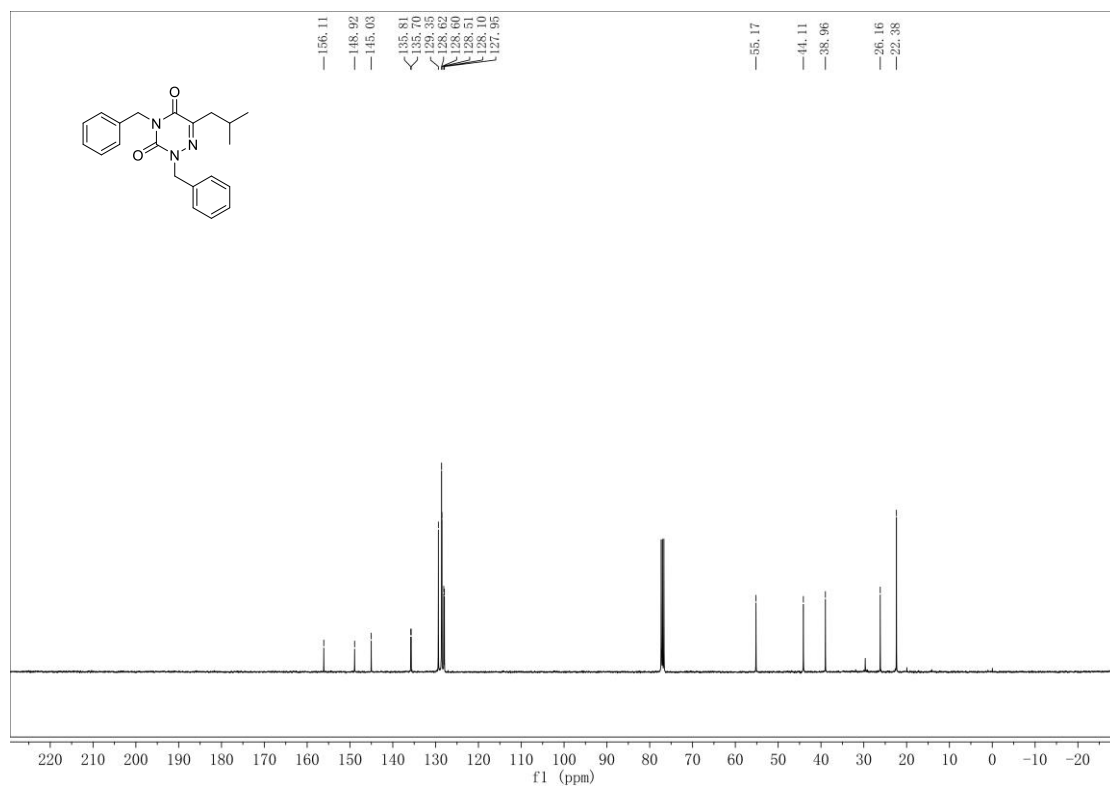
3p-¹³C

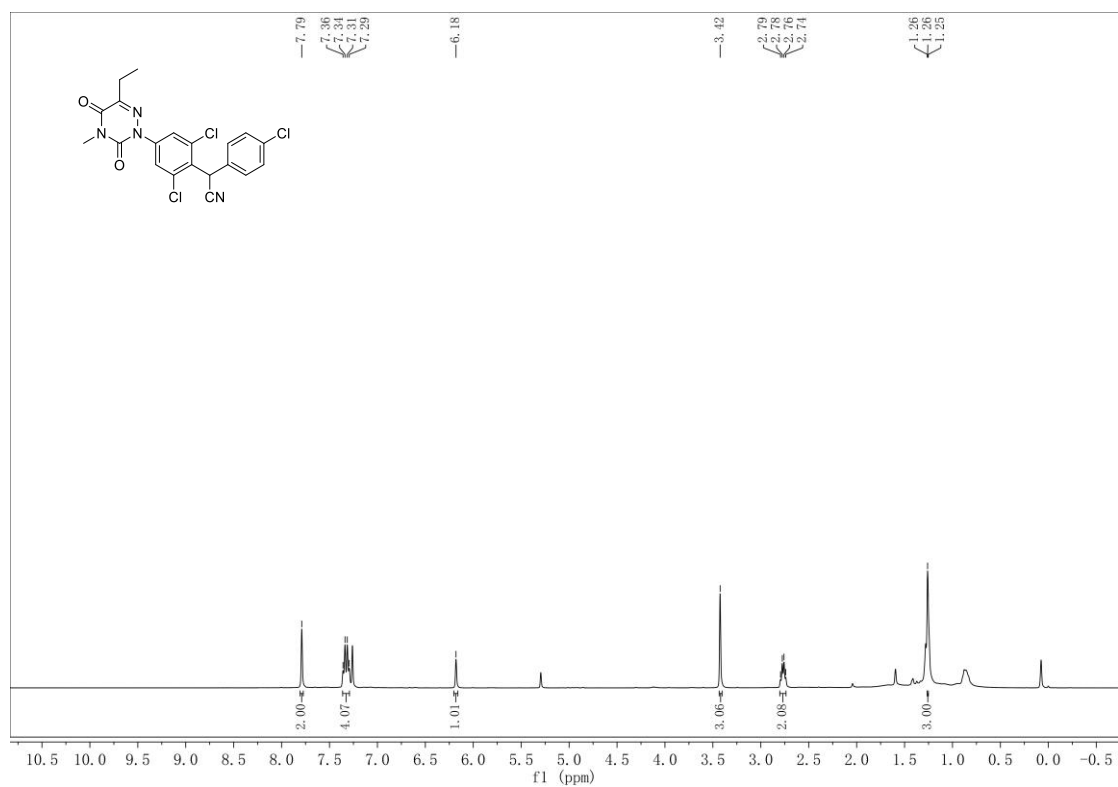
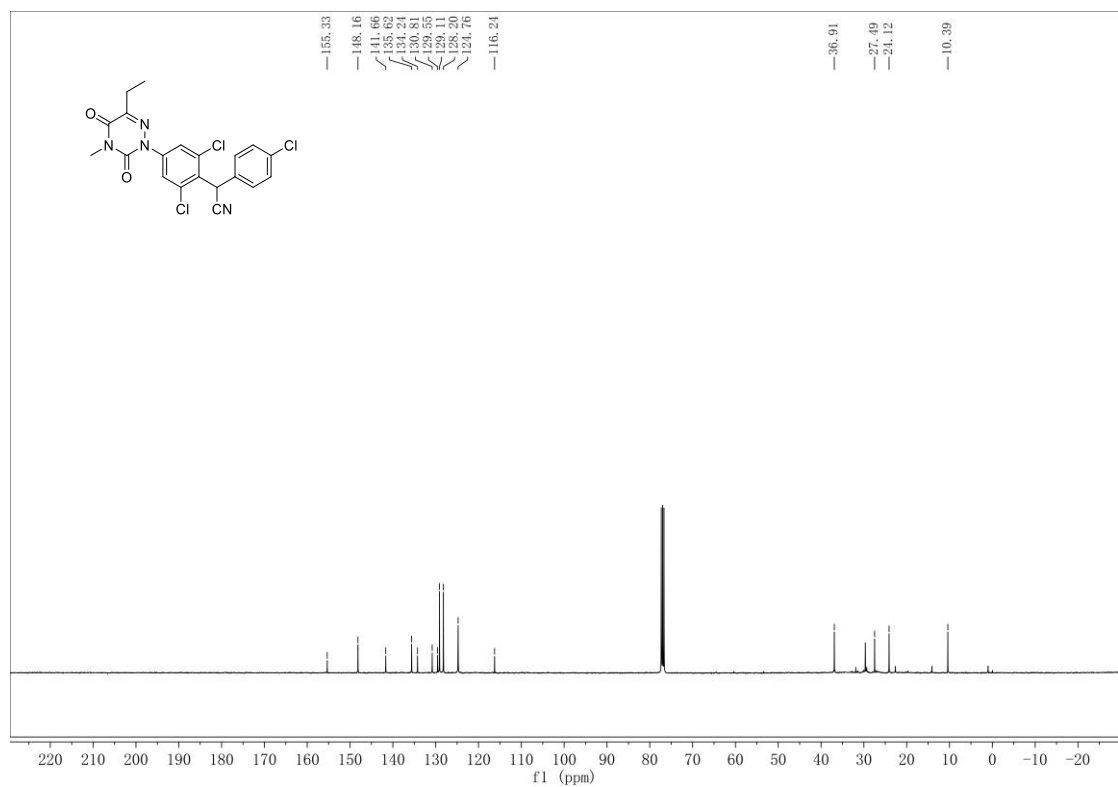


3q-¹H

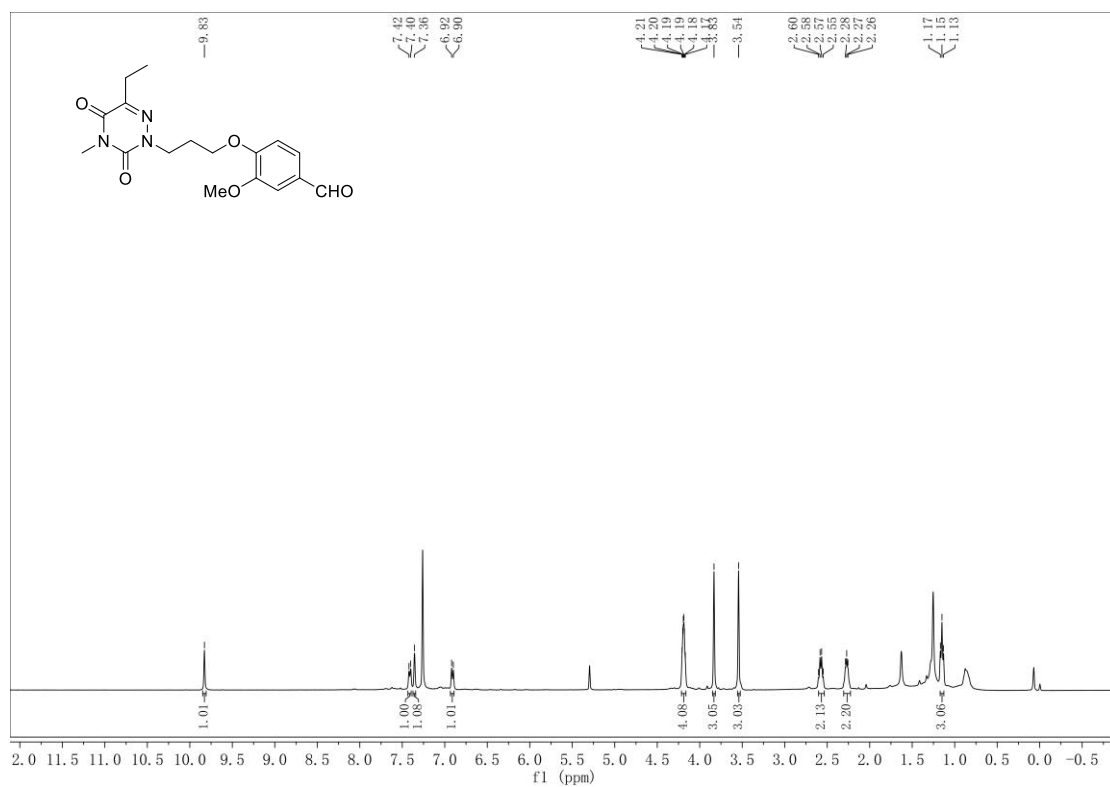


3q-¹³C

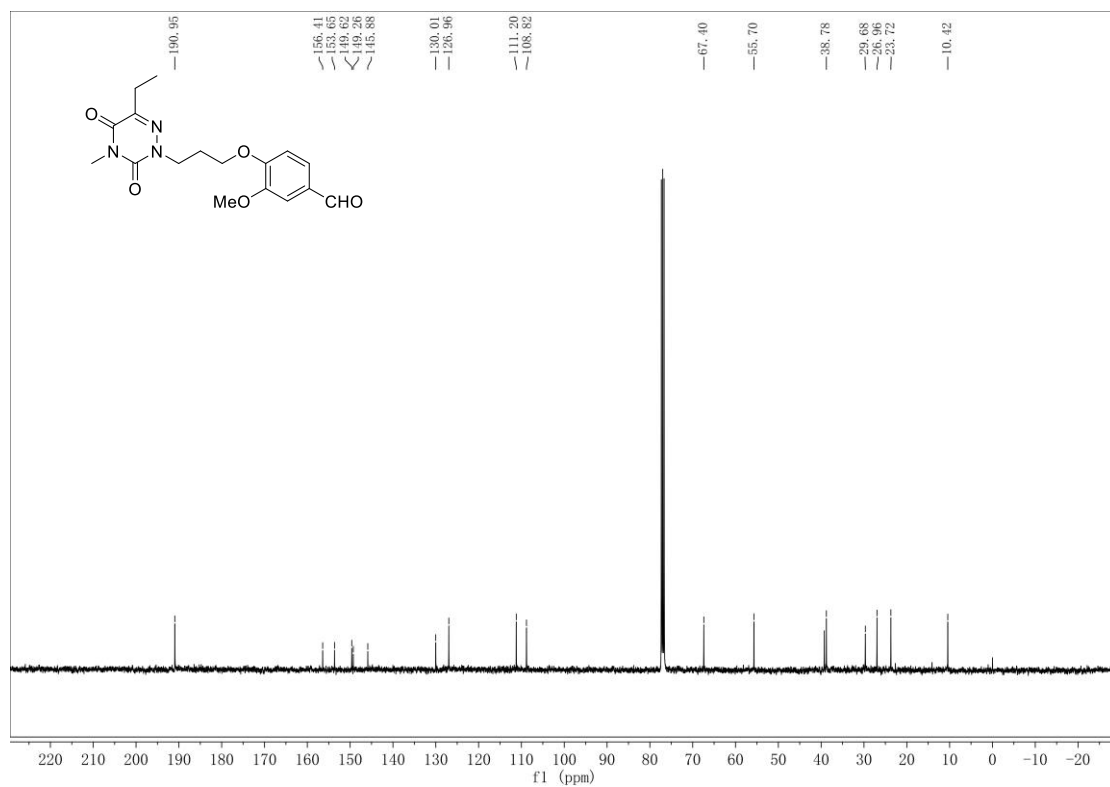


3r-¹H**3r-¹³C**

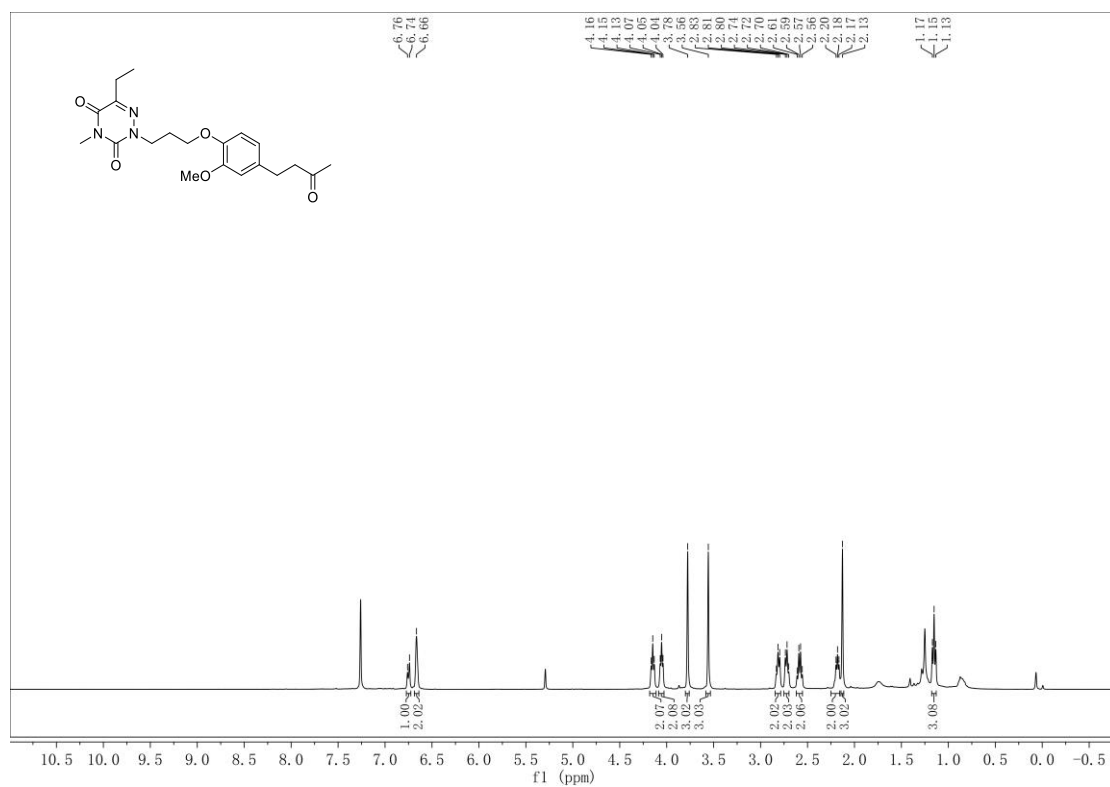
3s-¹H



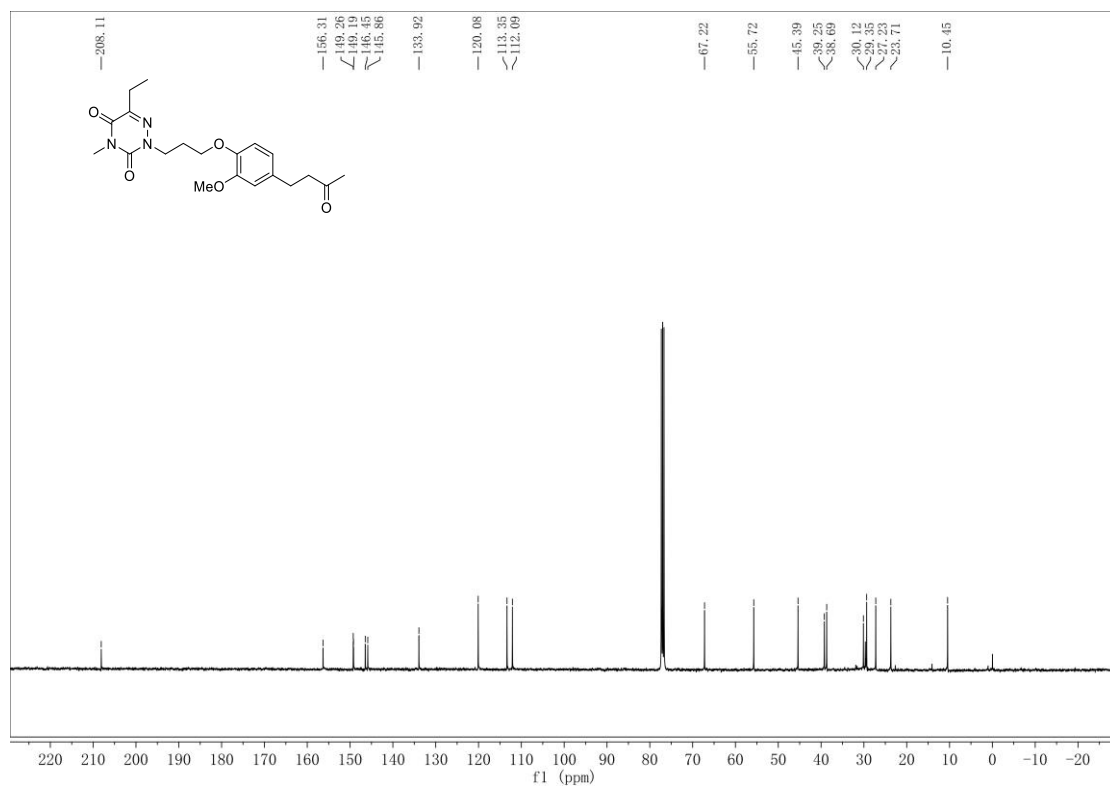
3s-¹³C



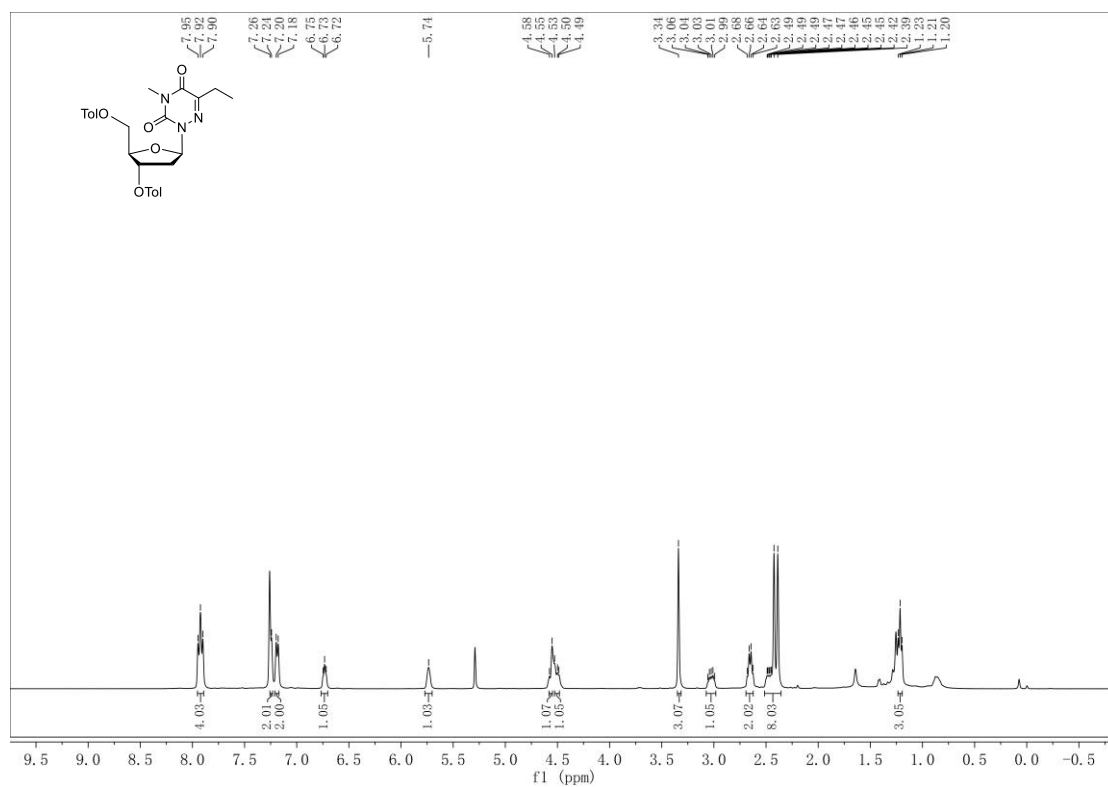
3t-¹H



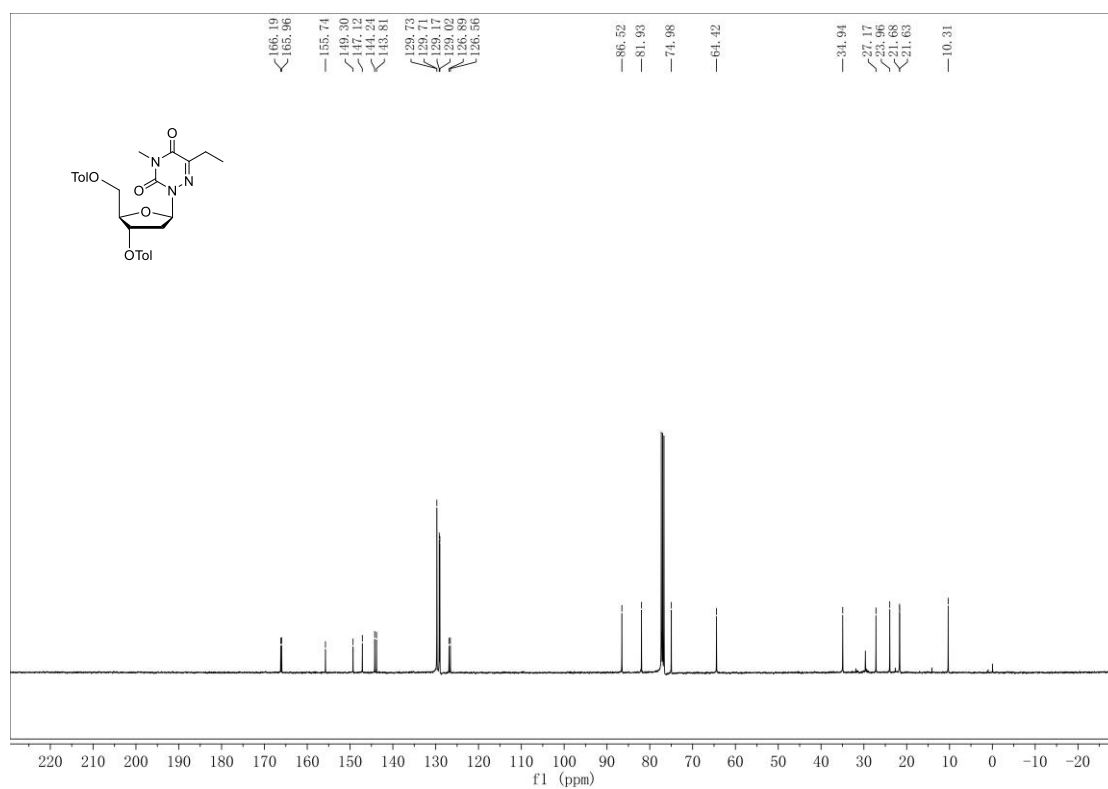
3t-¹³C

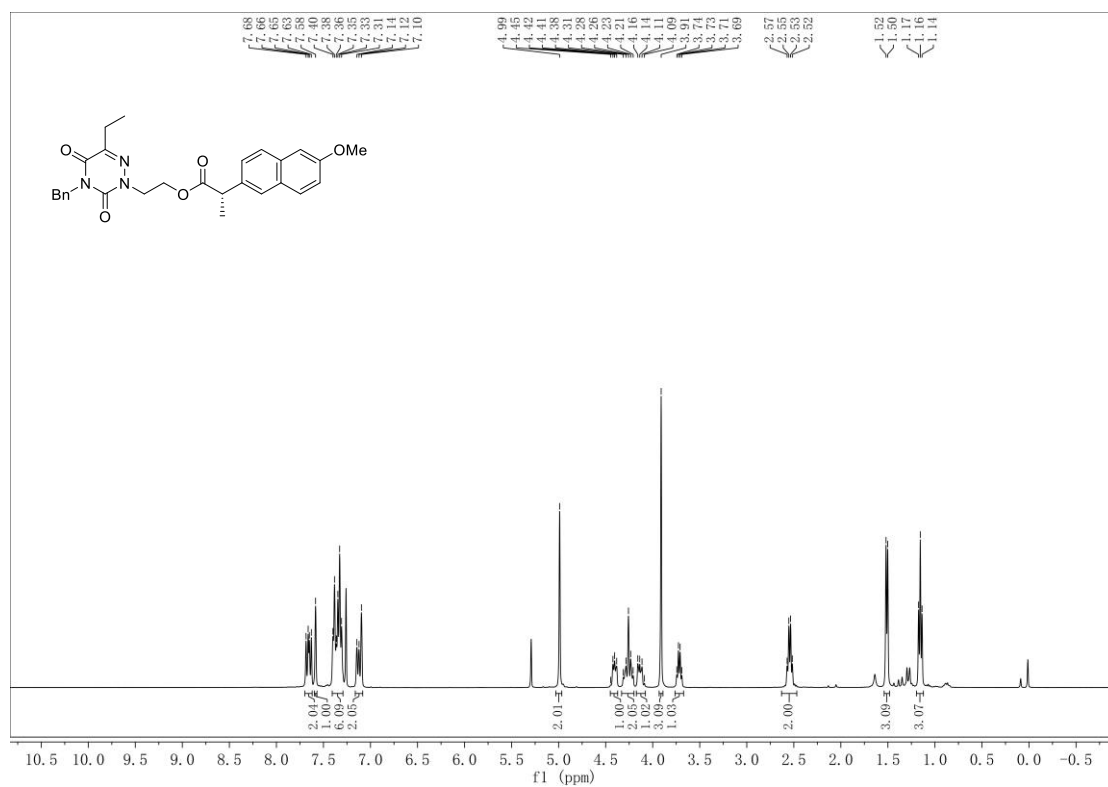
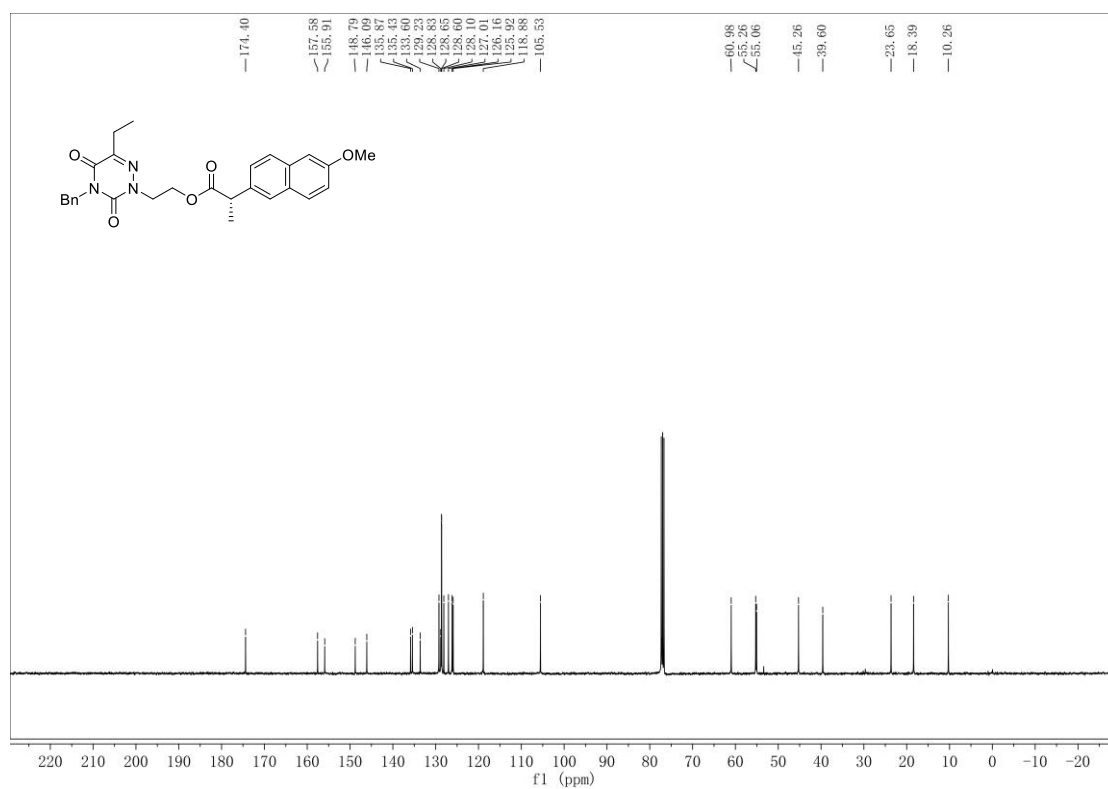


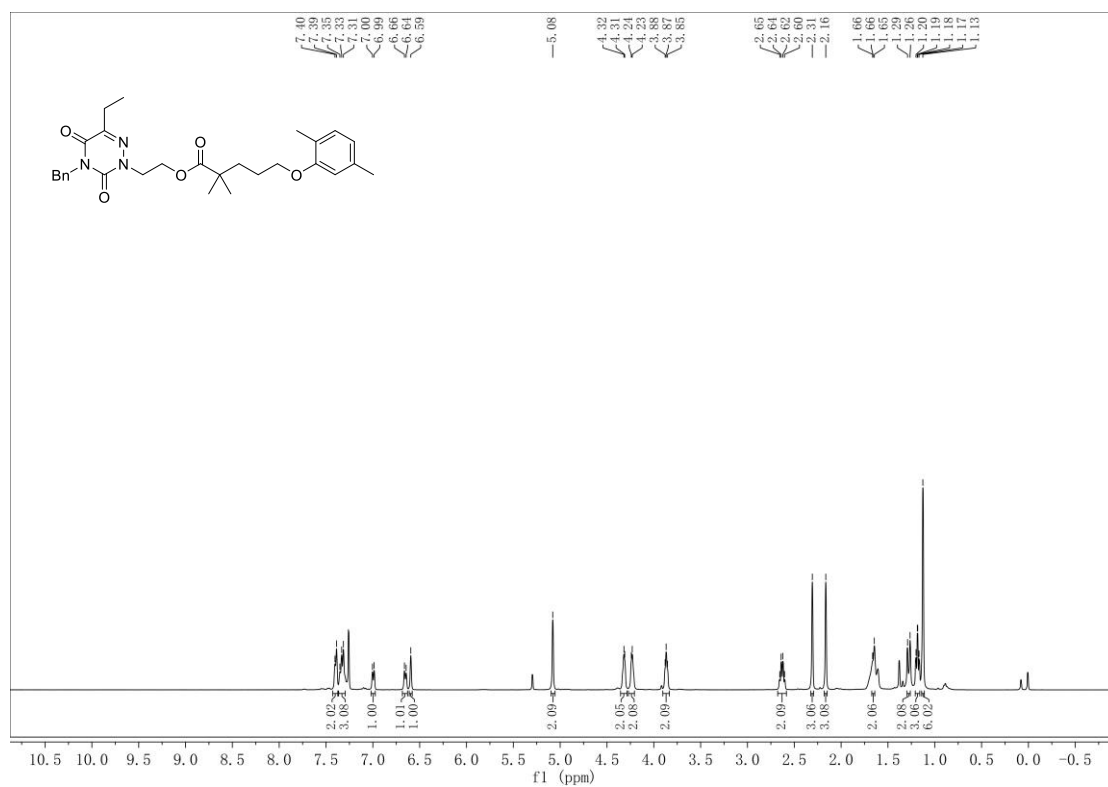
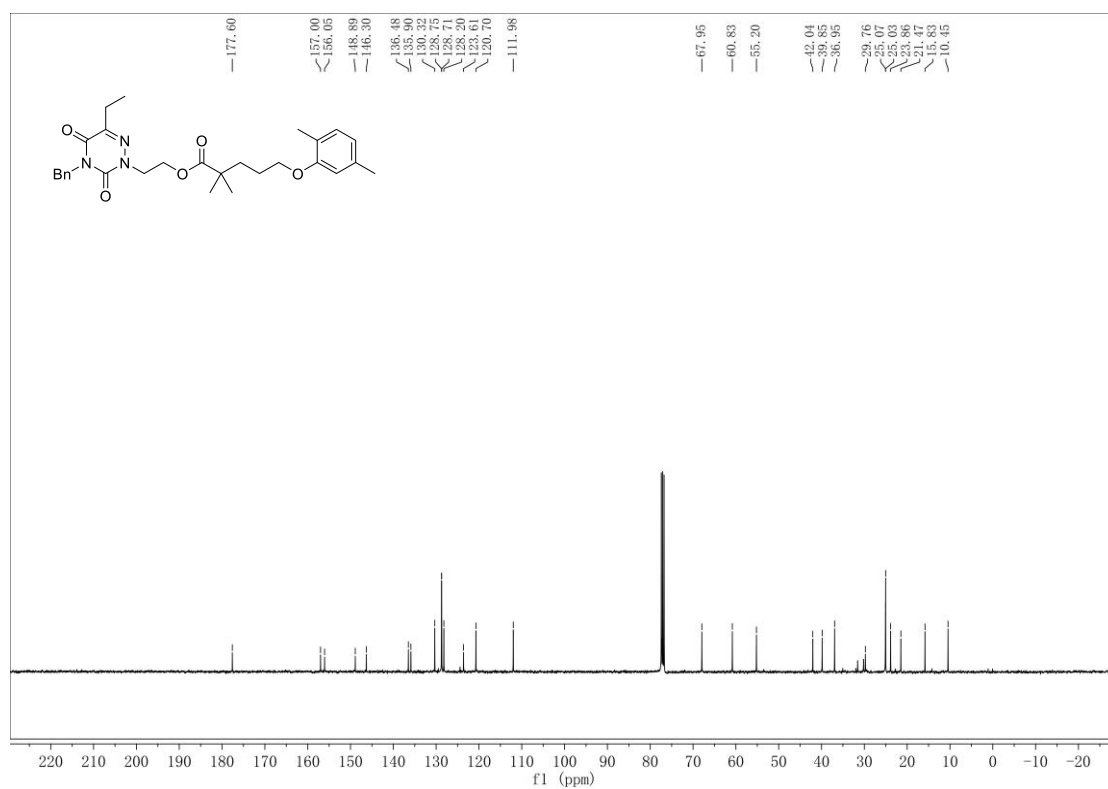
3u-¹H



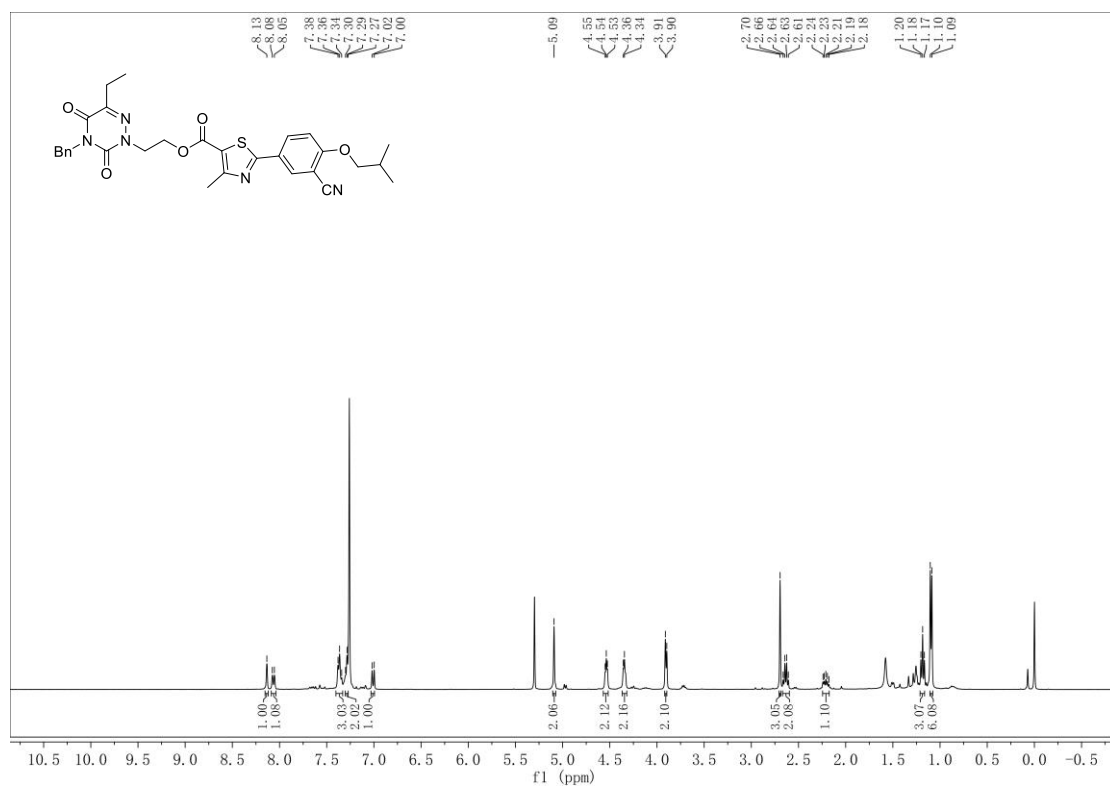
3u-¹³C



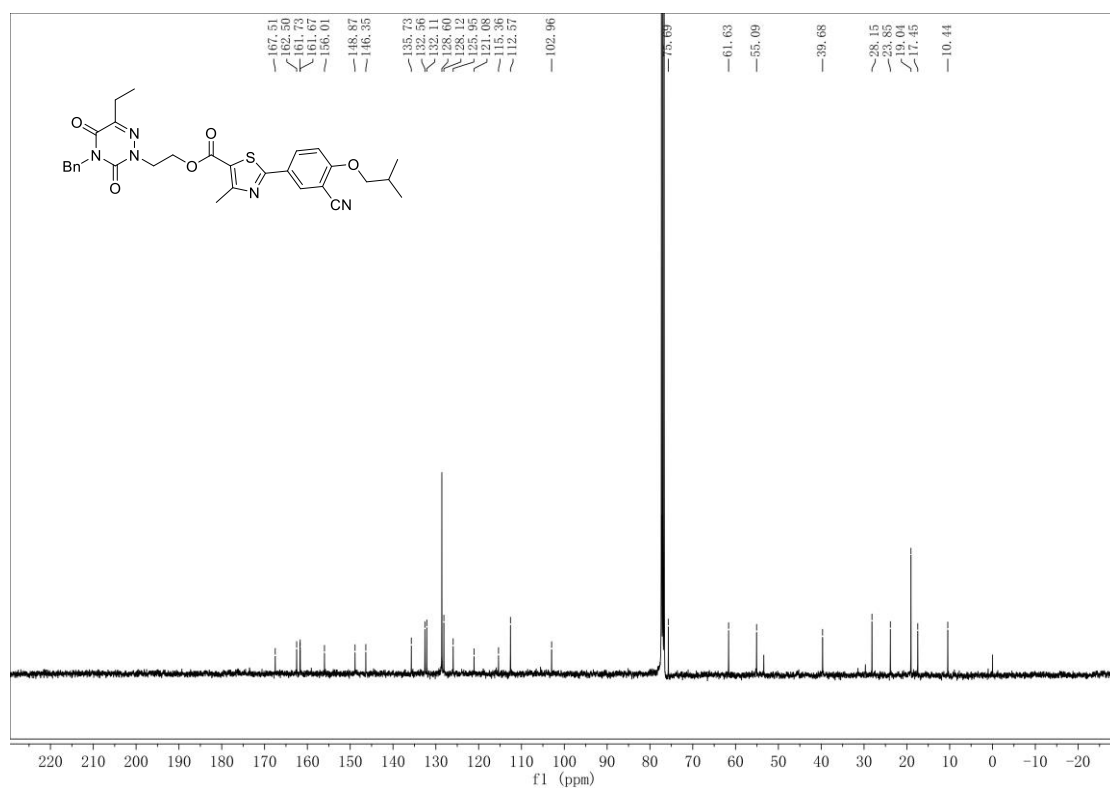
3v-¹H**3v-¹³C**

3w-¹H**3w-¹³C**

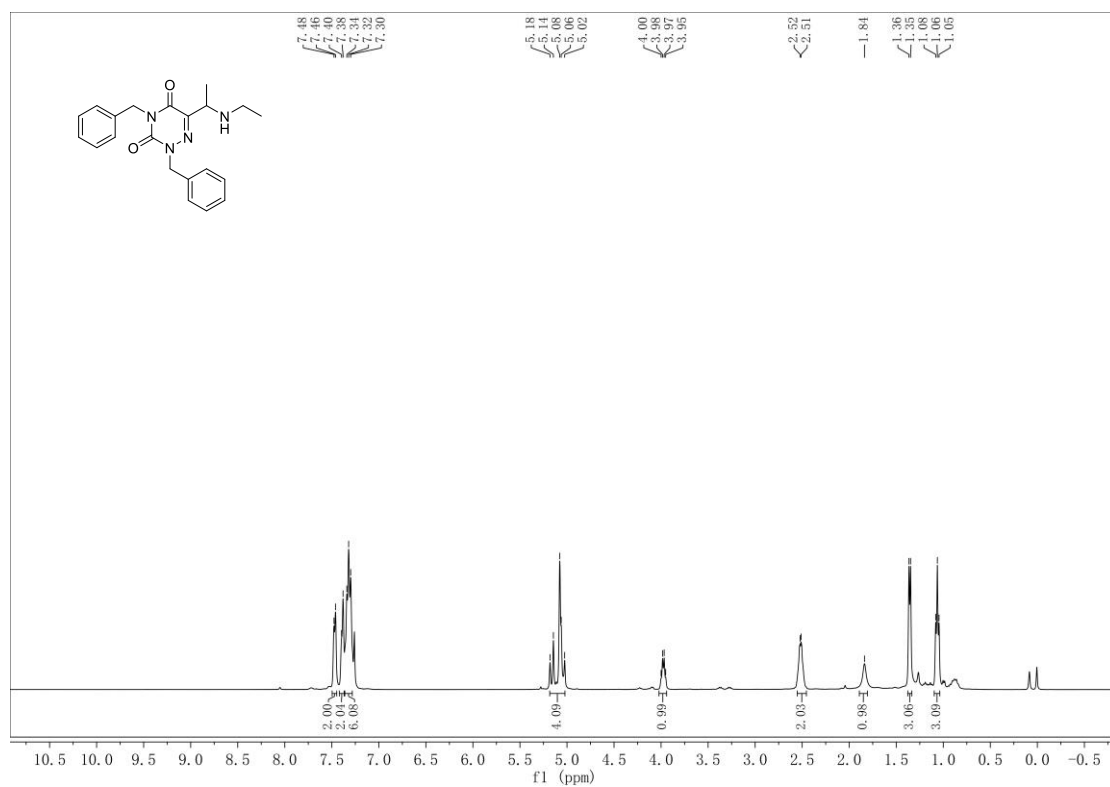
3x-¹H



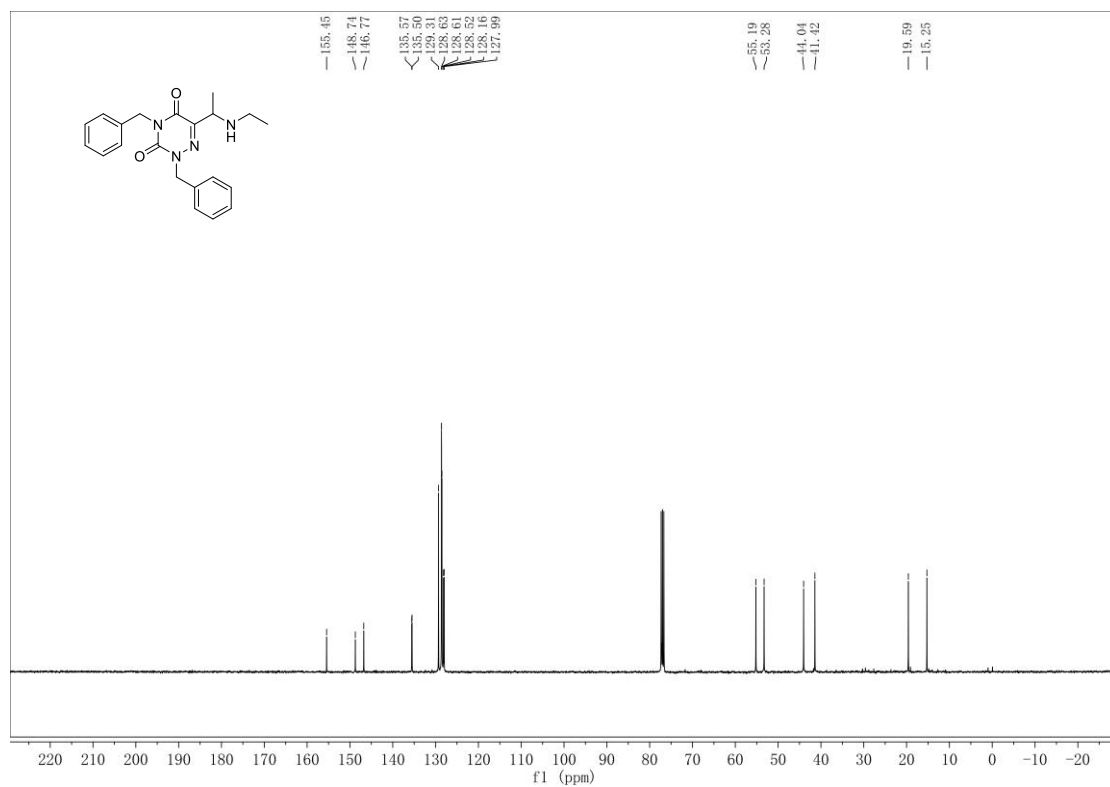
3x-¹³C



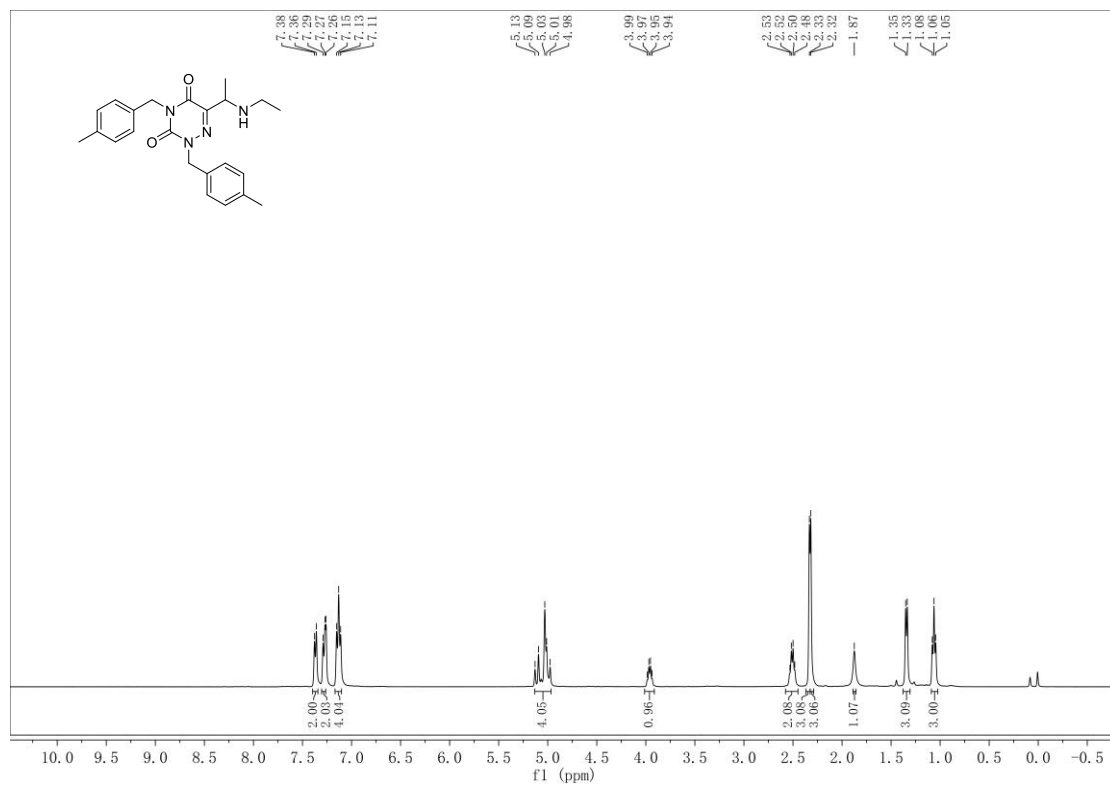
4a-¹H



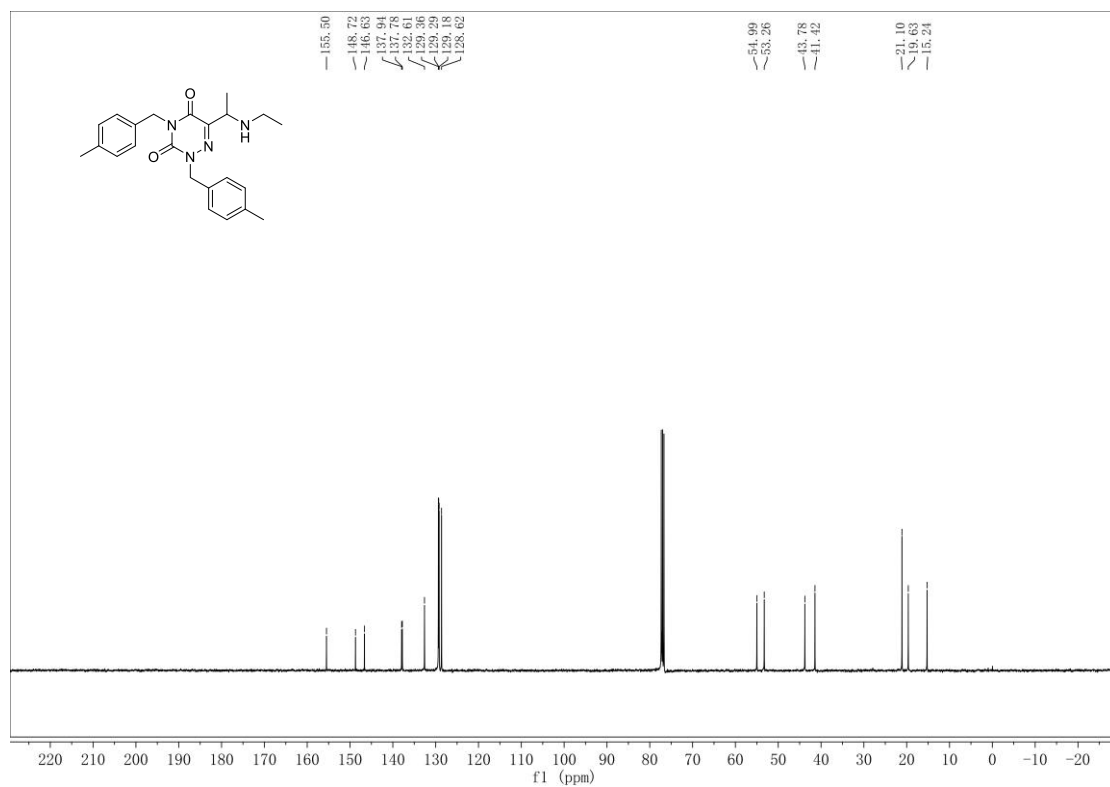
4a-¹³C

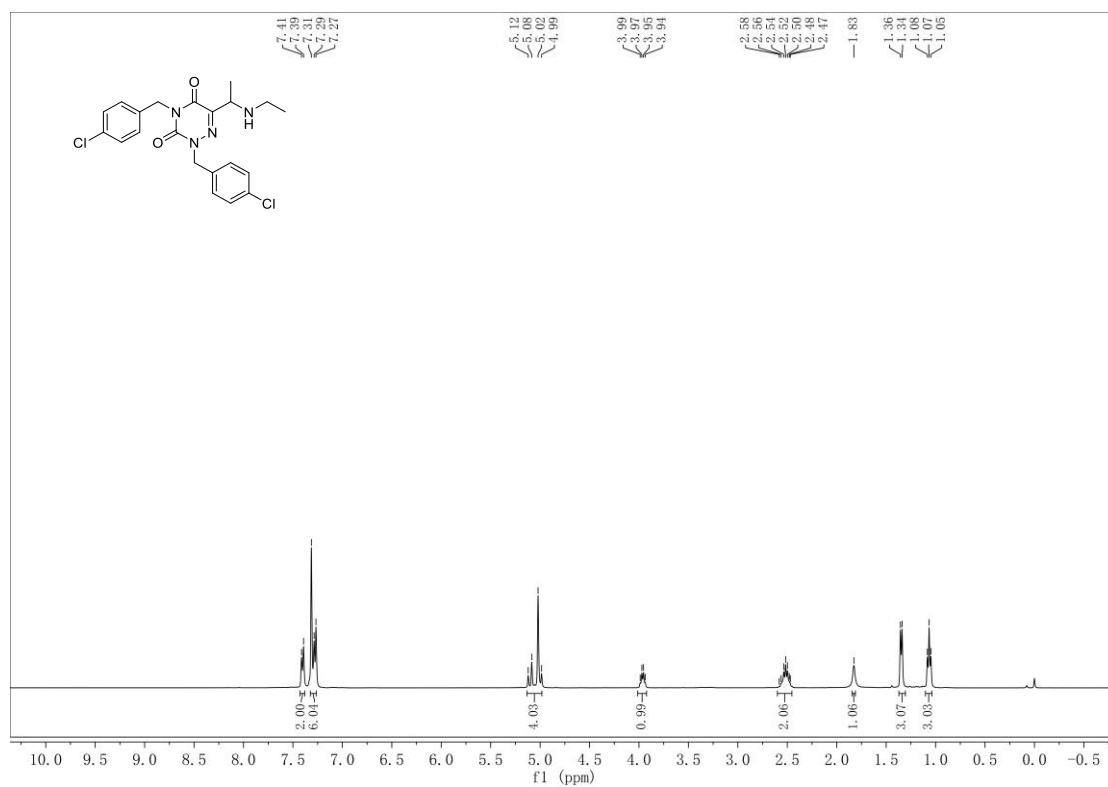
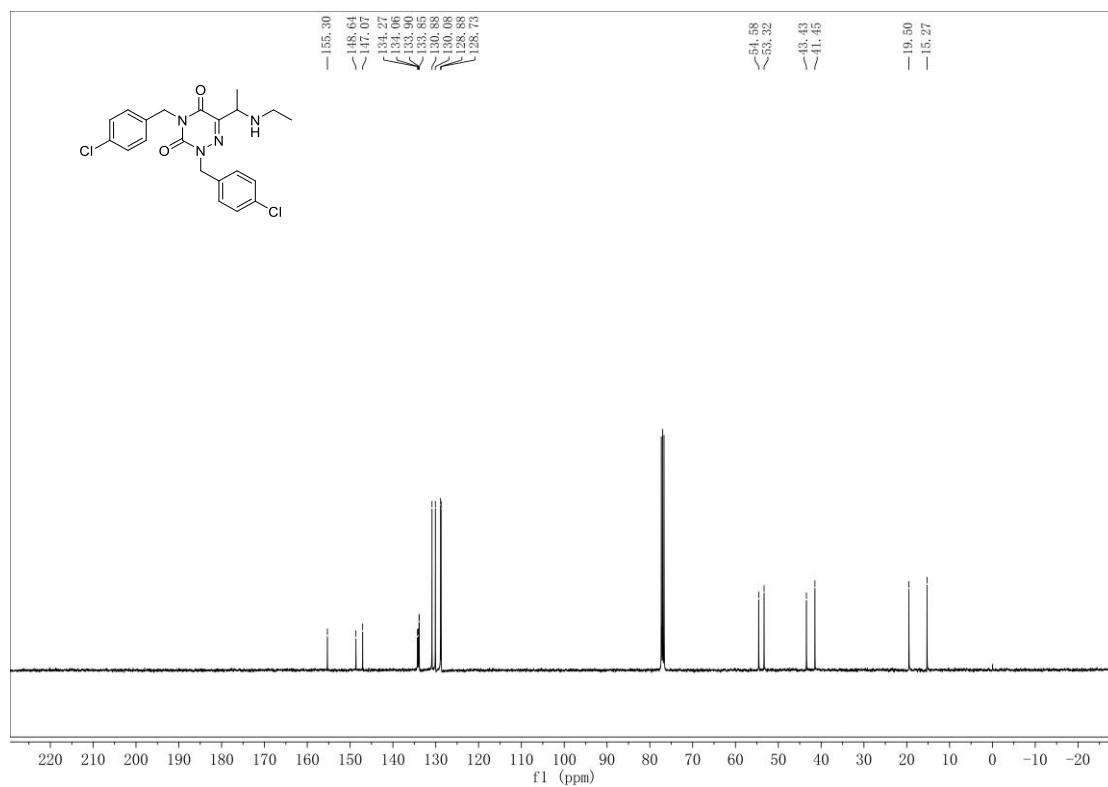


4b-¹H

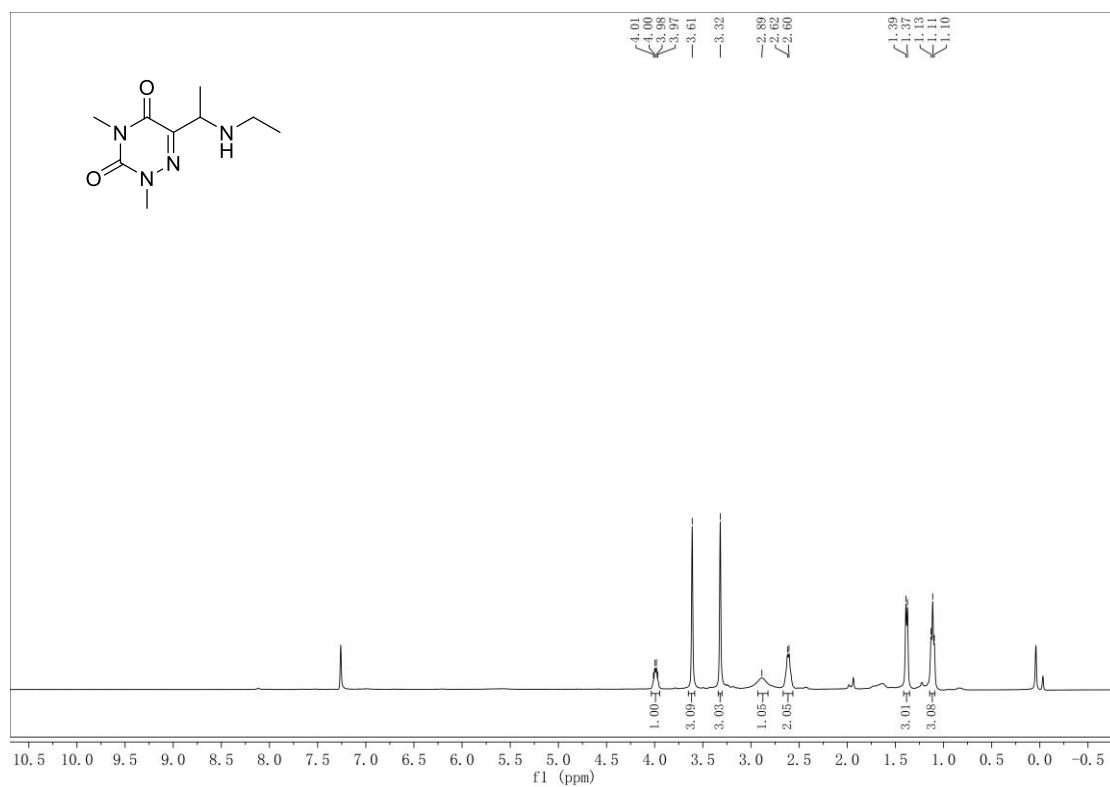


4b-¹³C

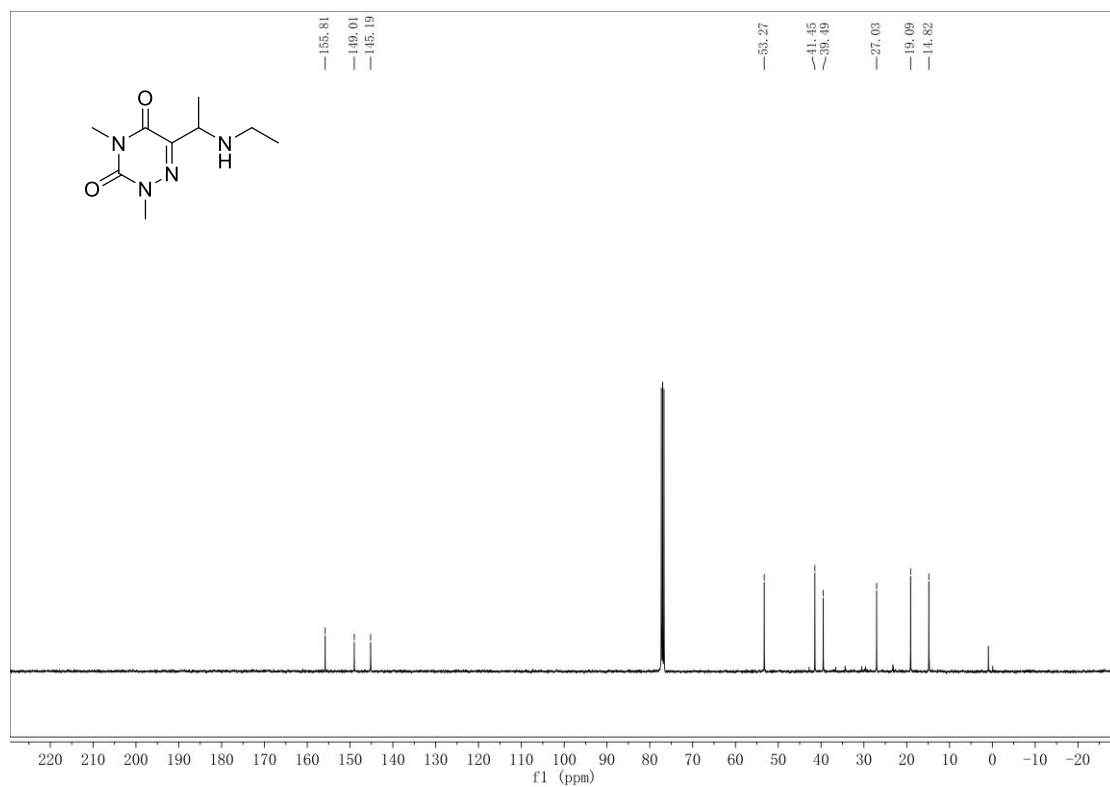


4c-¹H**4c-¹³C**

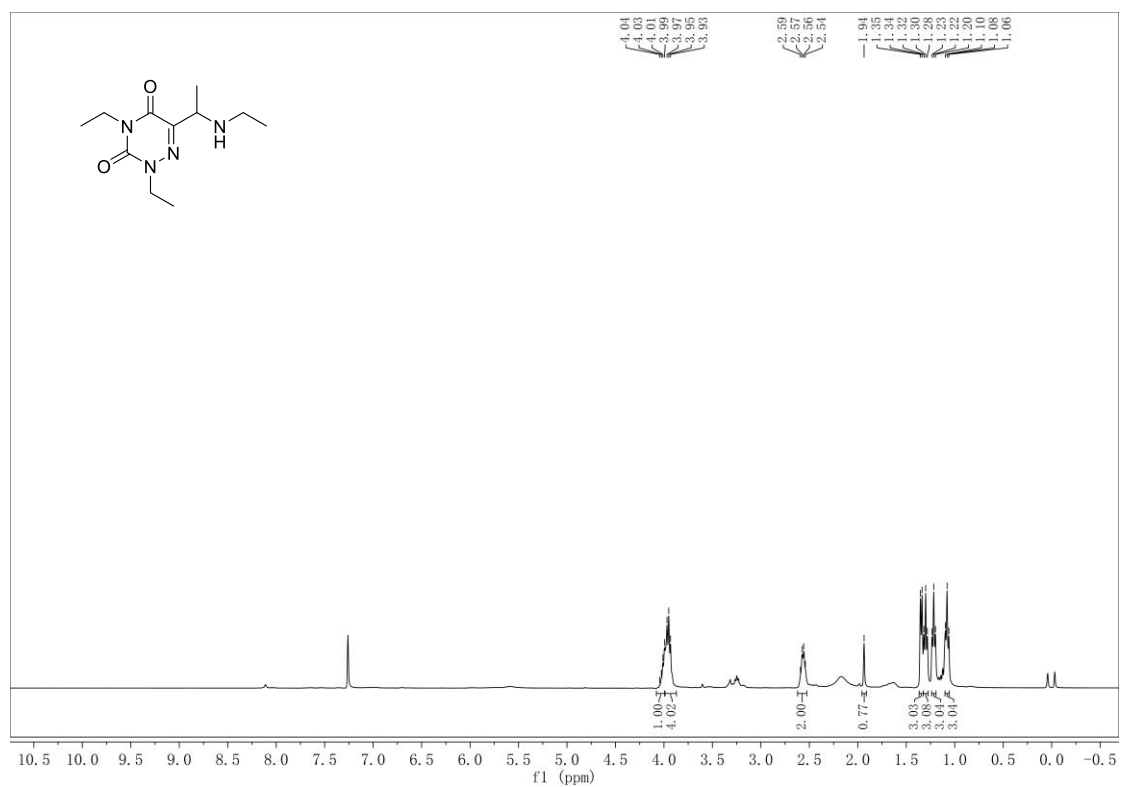
4d-¹H



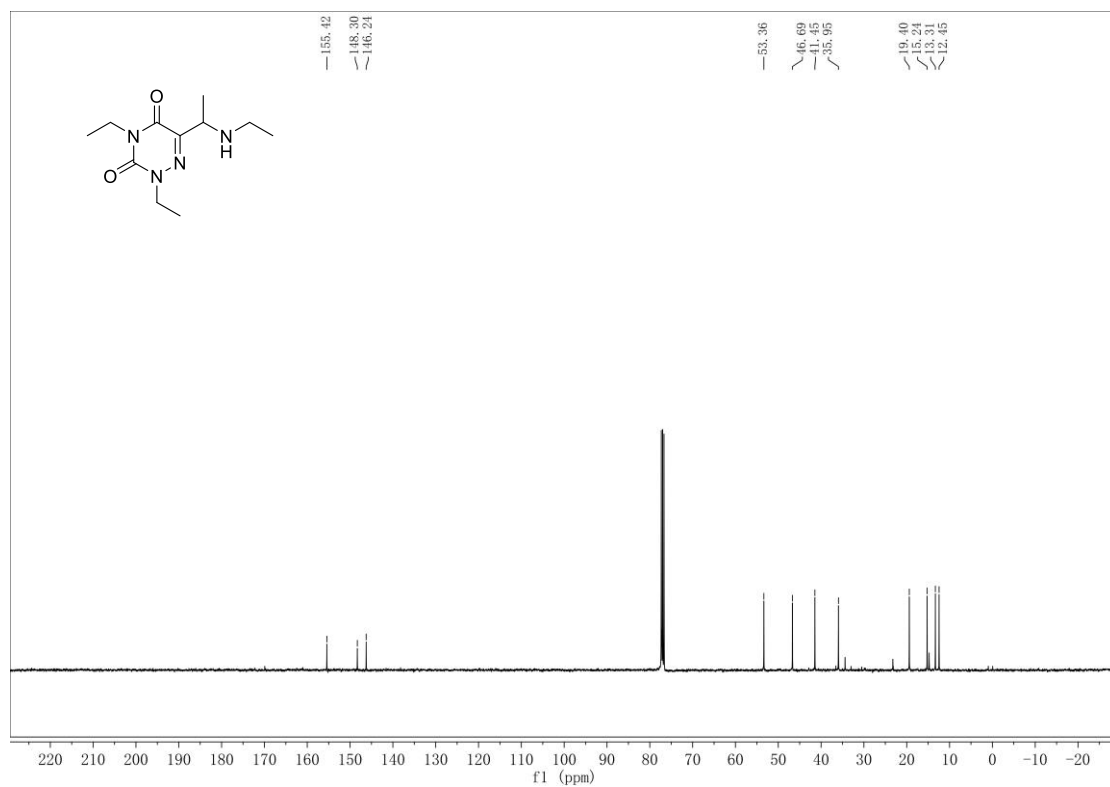
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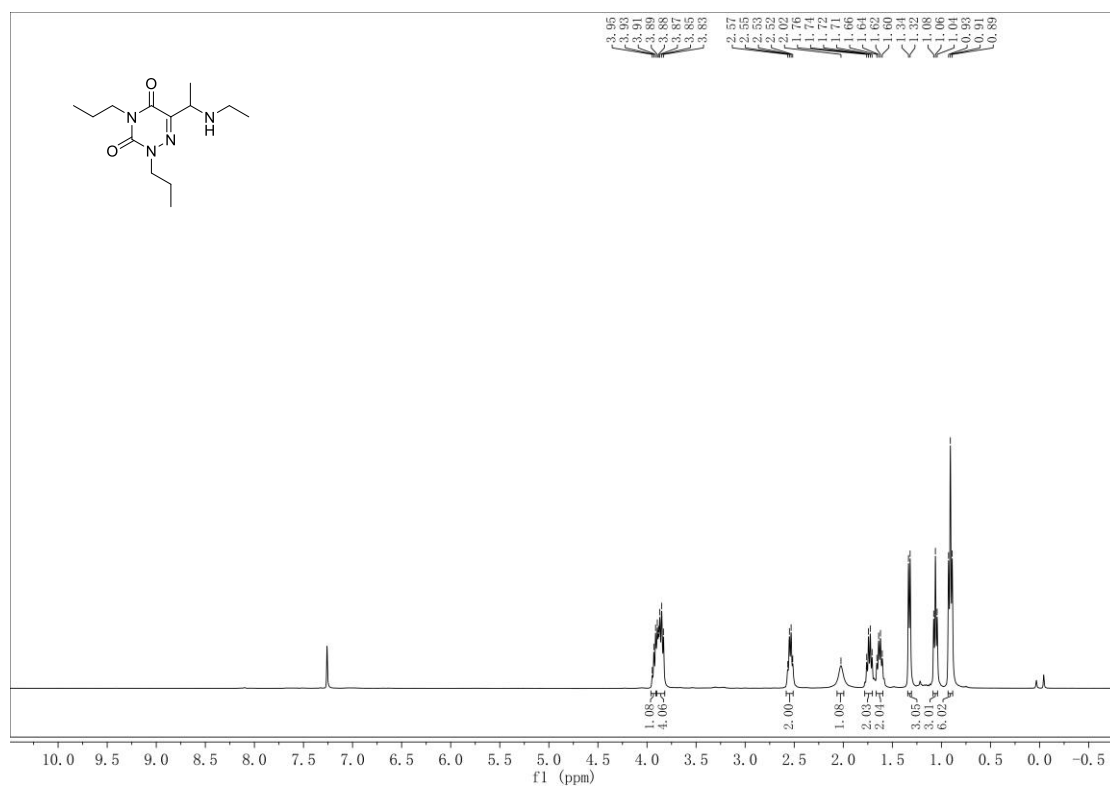
4e-¹H



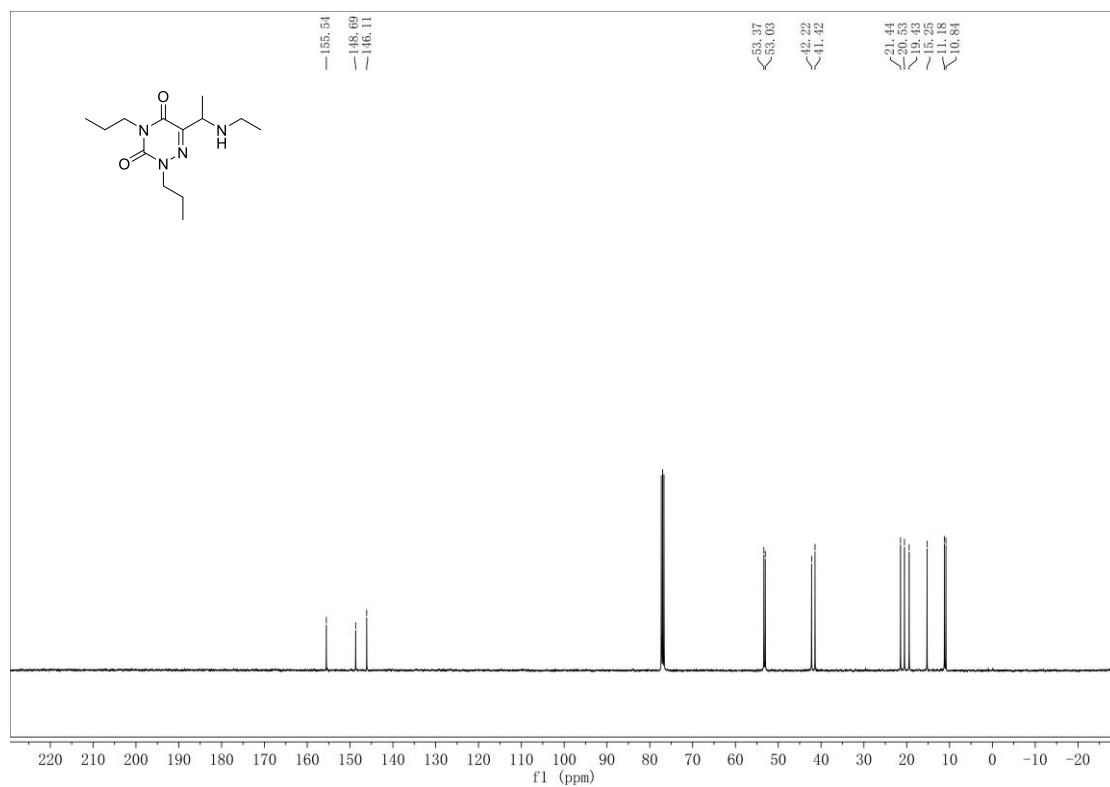
4e-¹³C



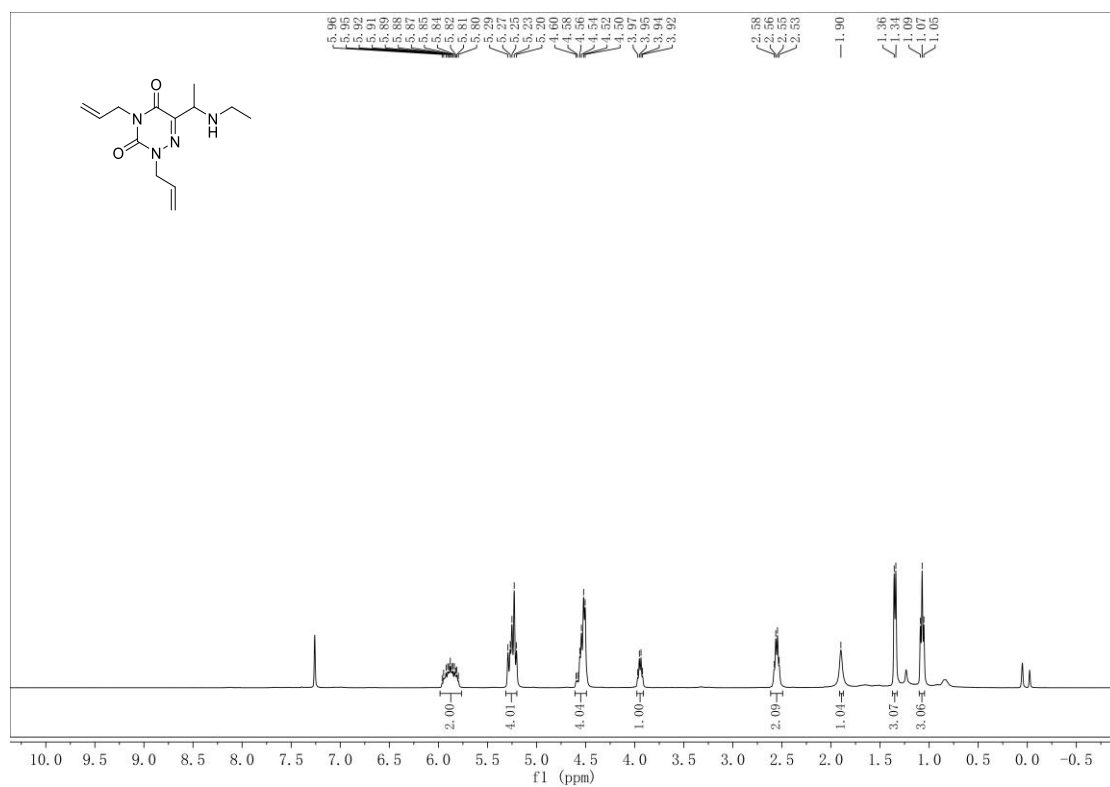
4f-¹H



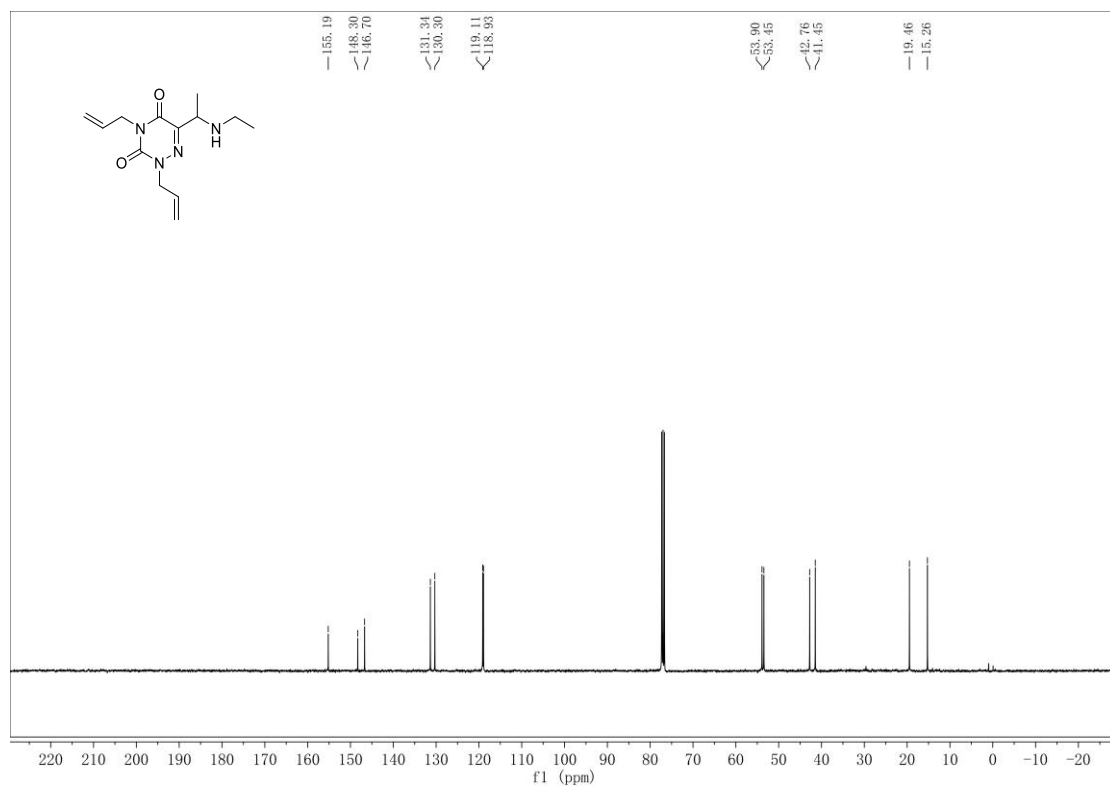
4f-¹³C



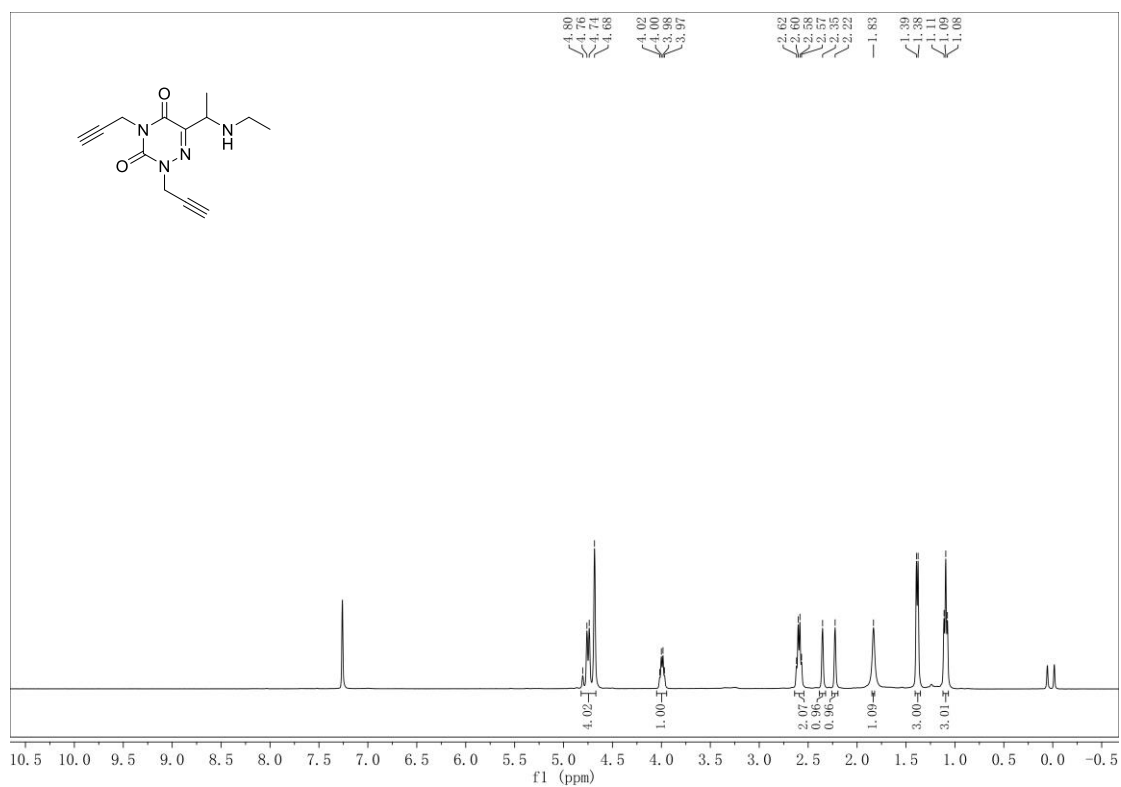
4g-¹H



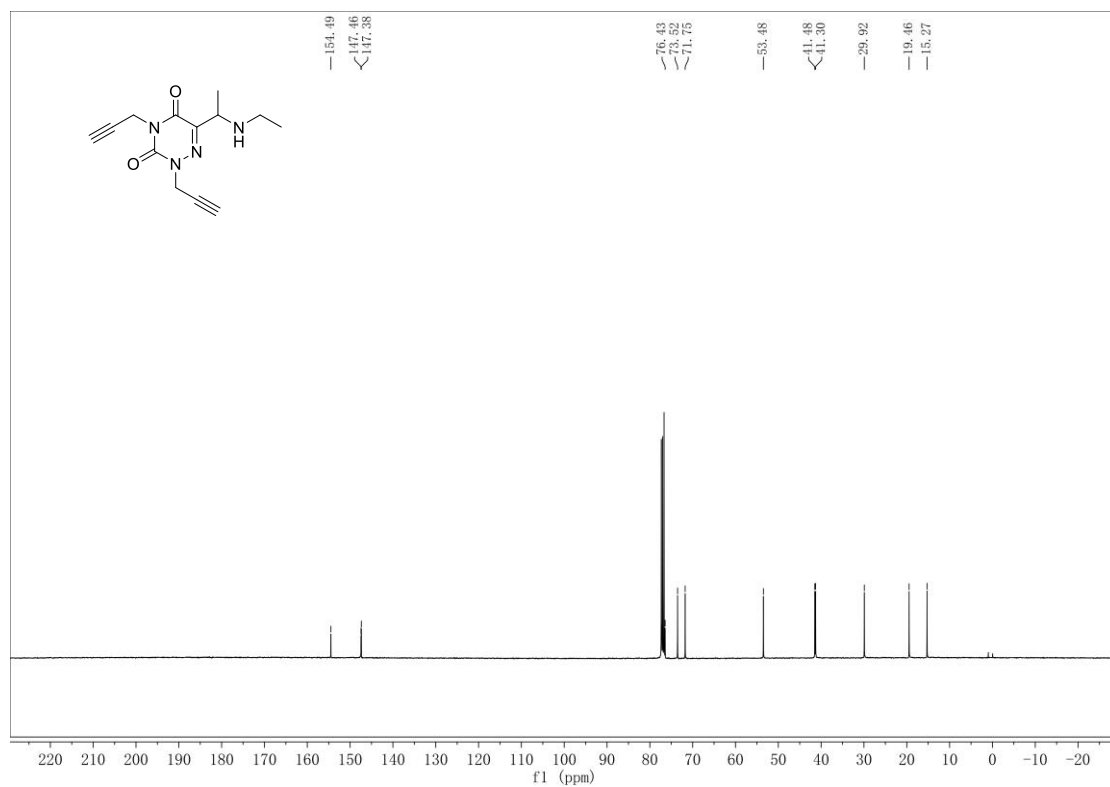
4g-¹³C



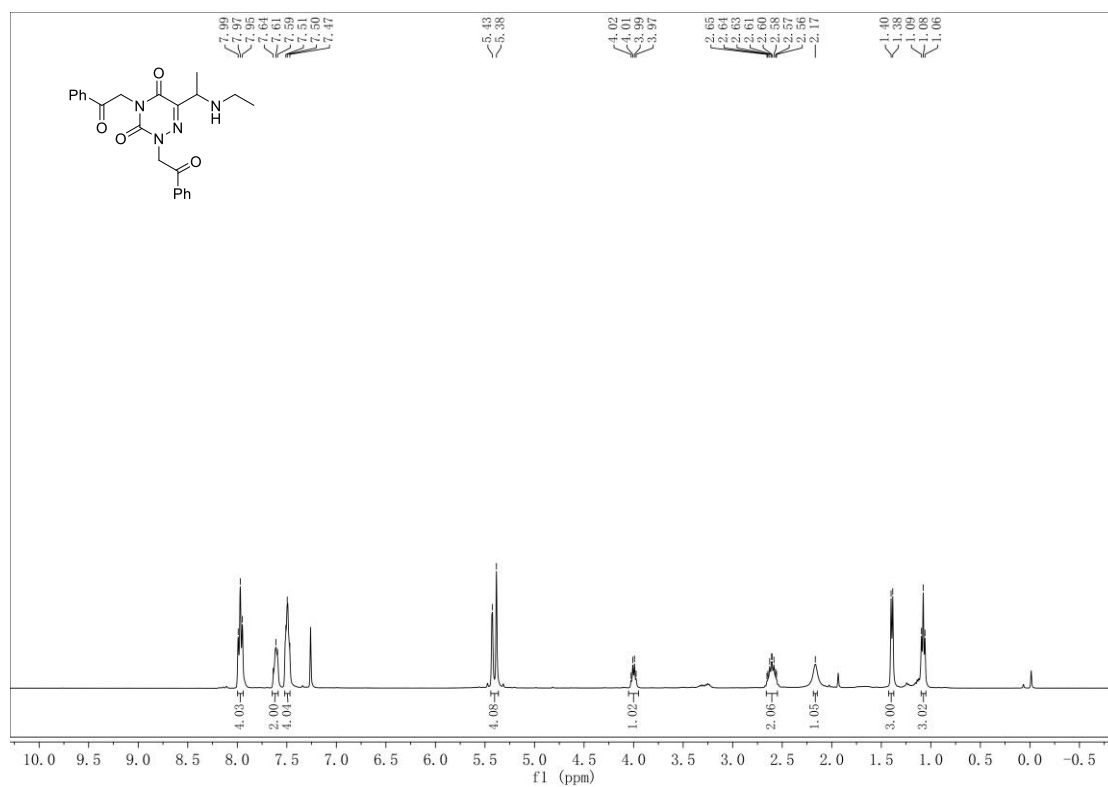
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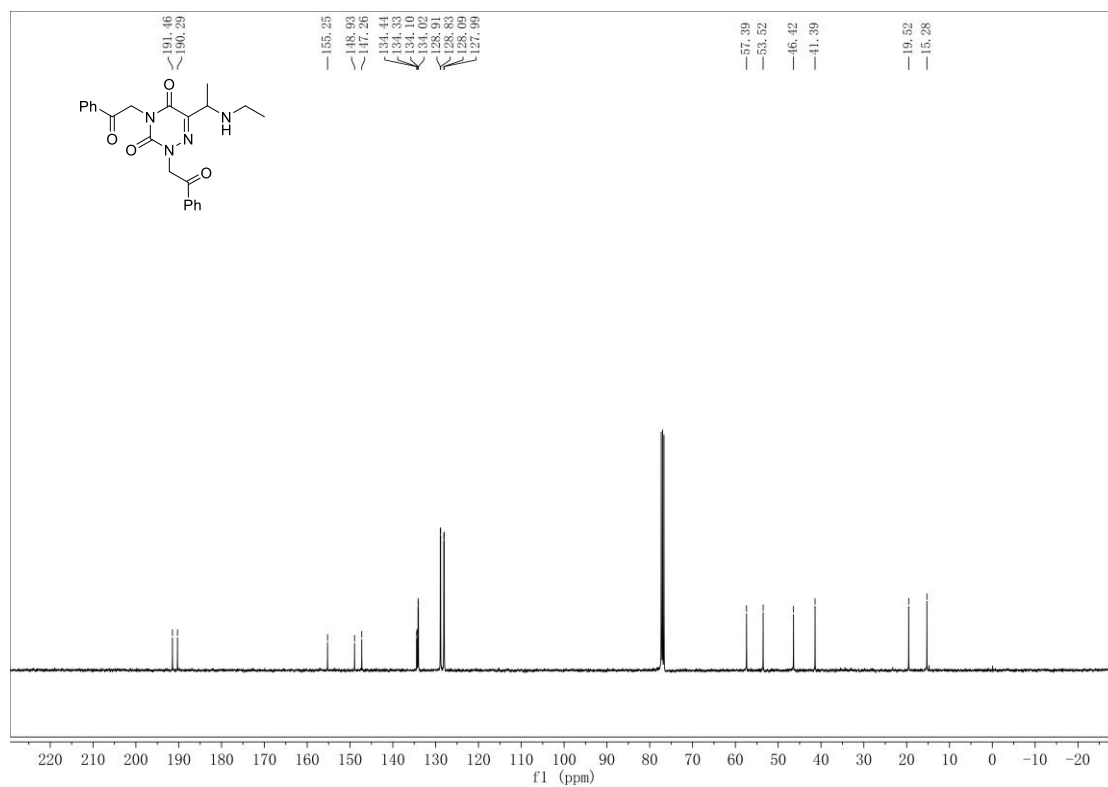
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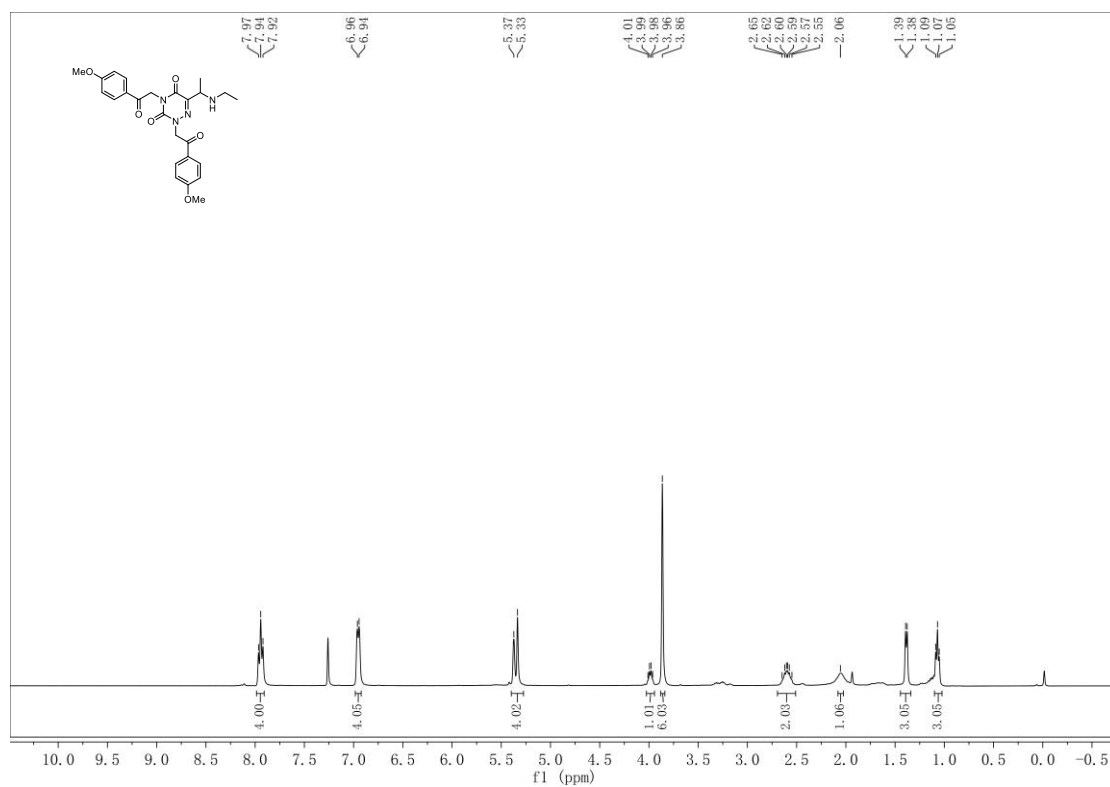
4i-¹H



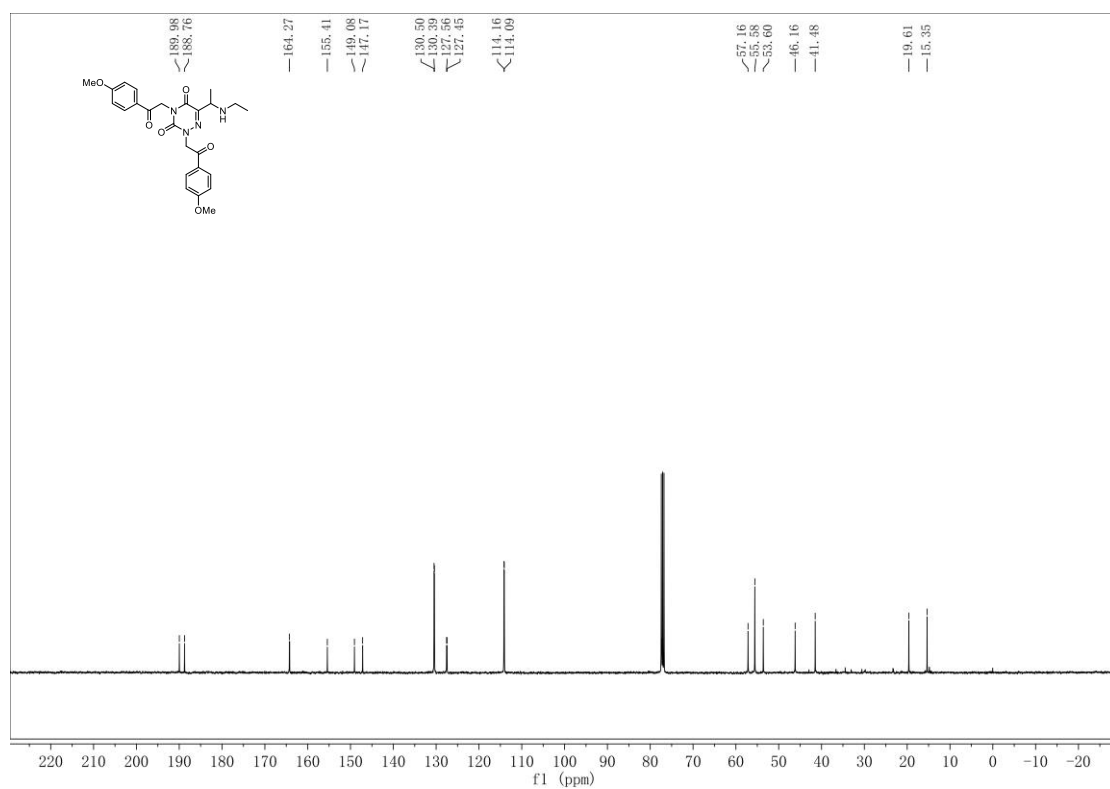
4i-¹³C



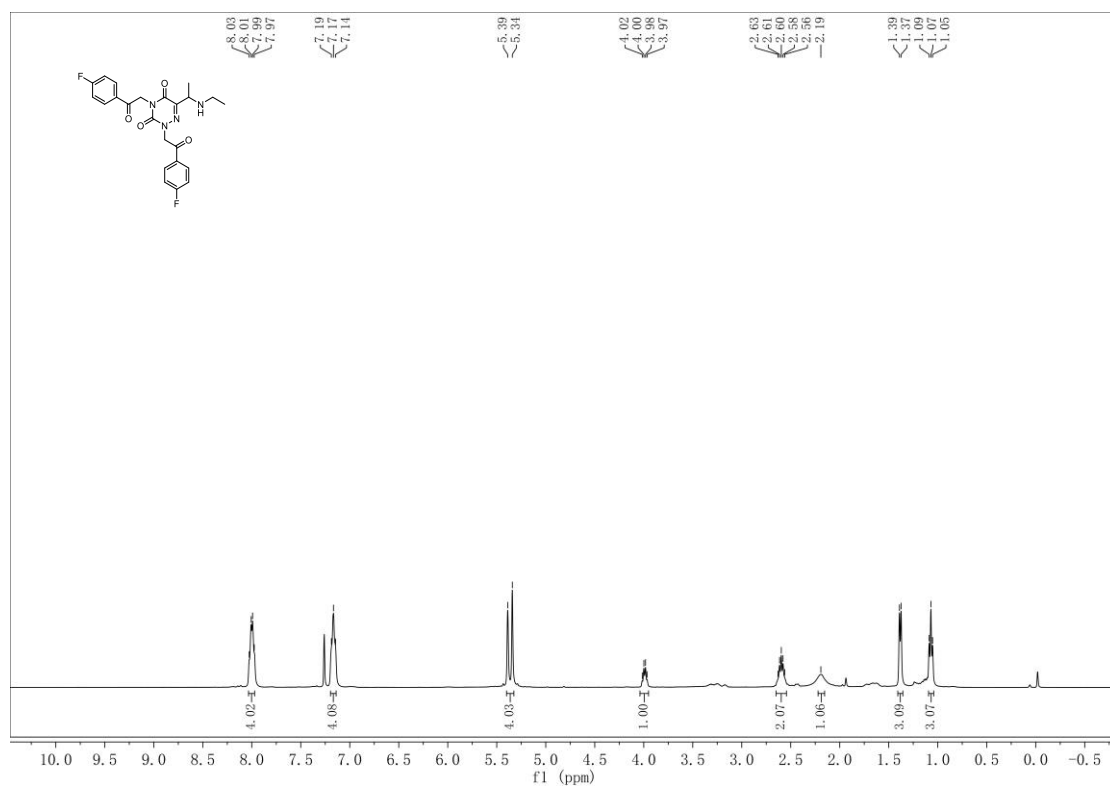
4j-¹H



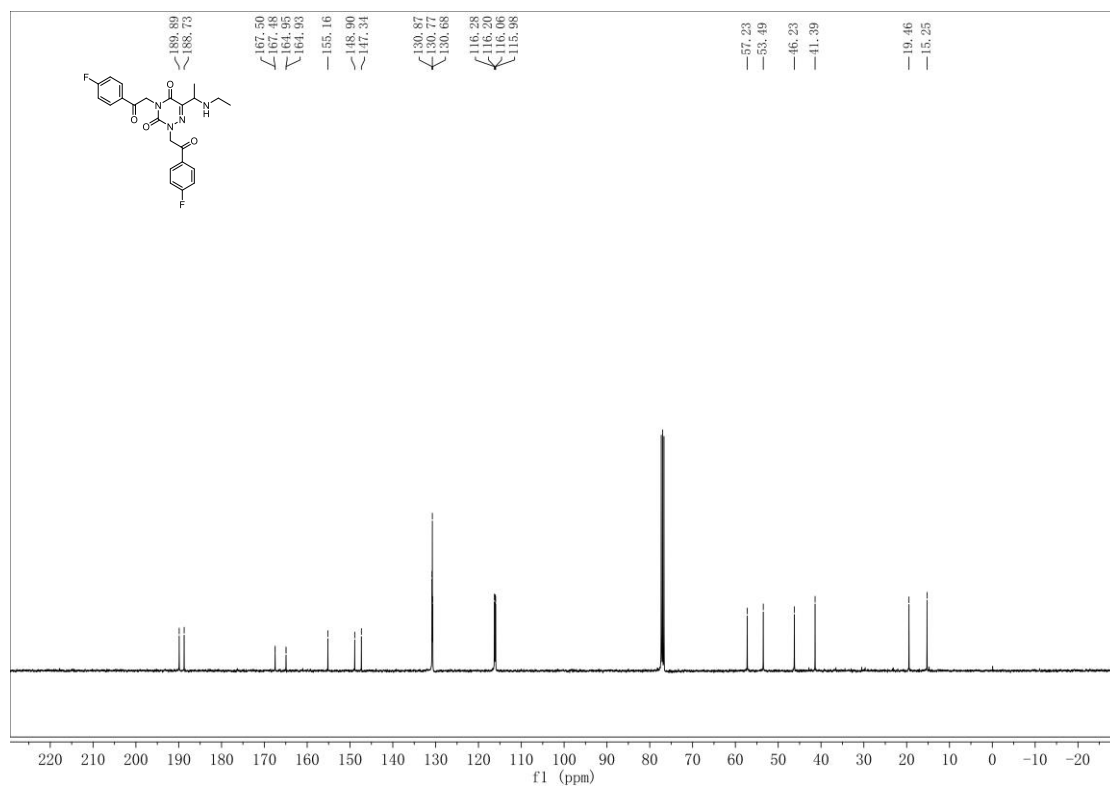
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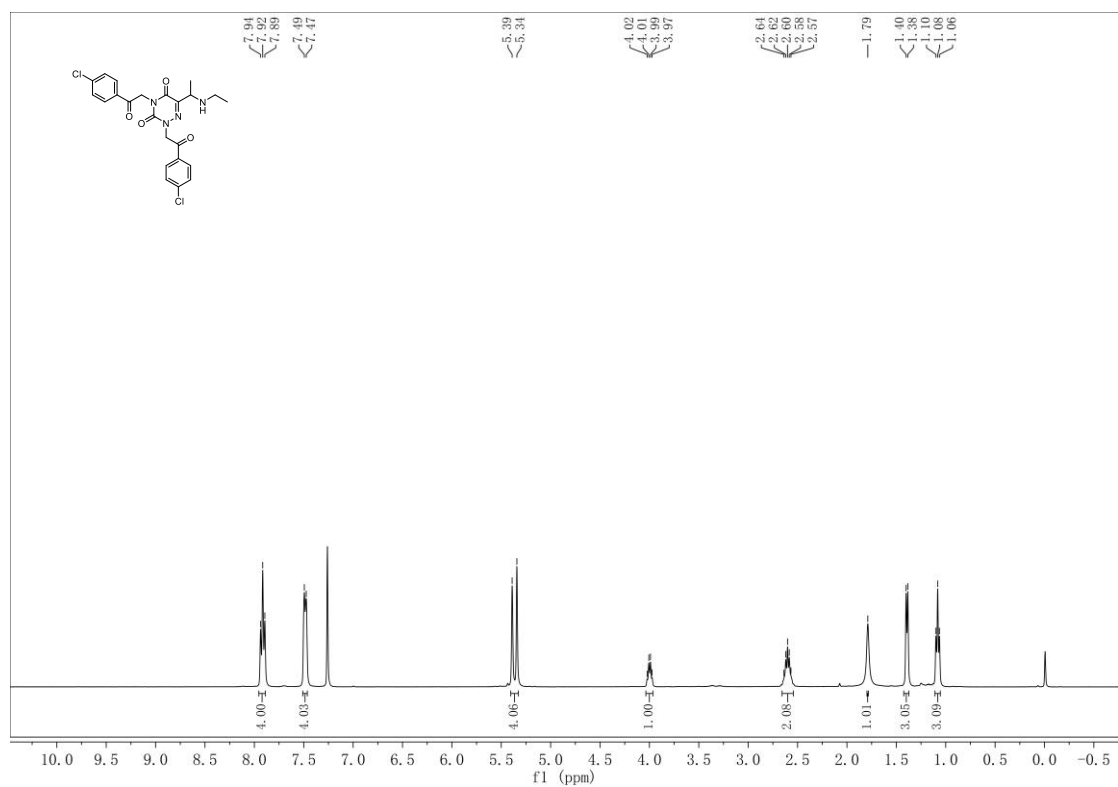
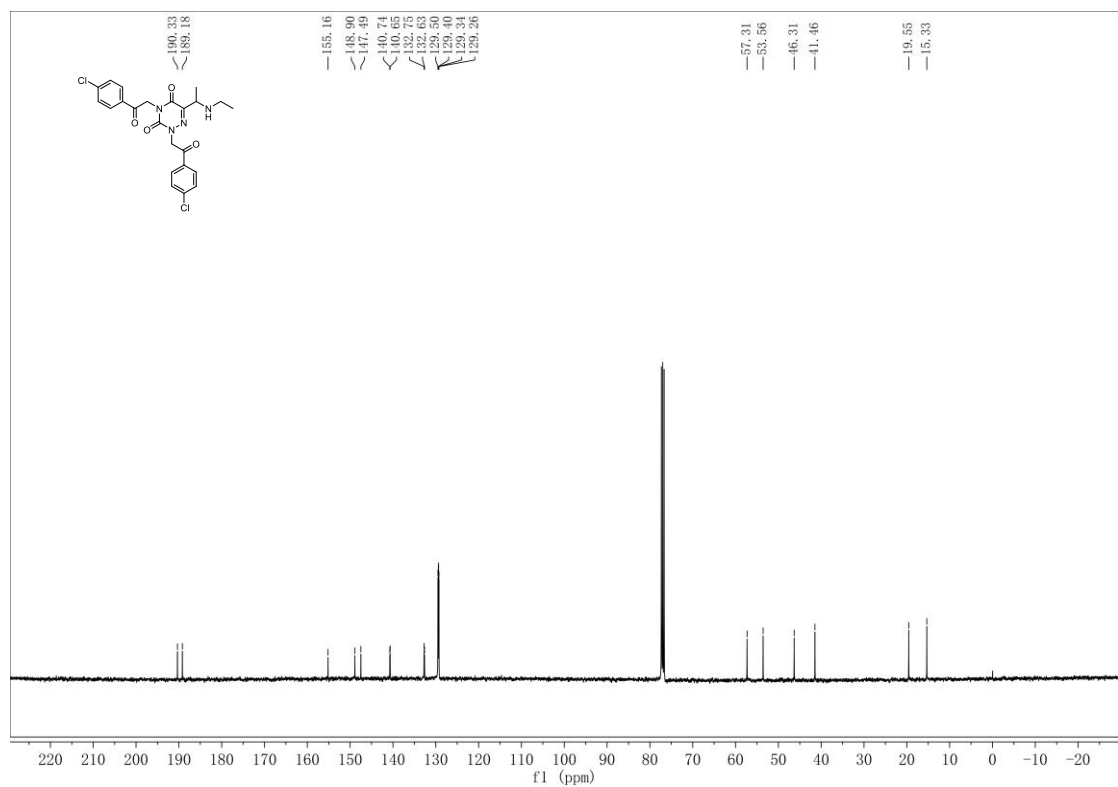


4k-¹H

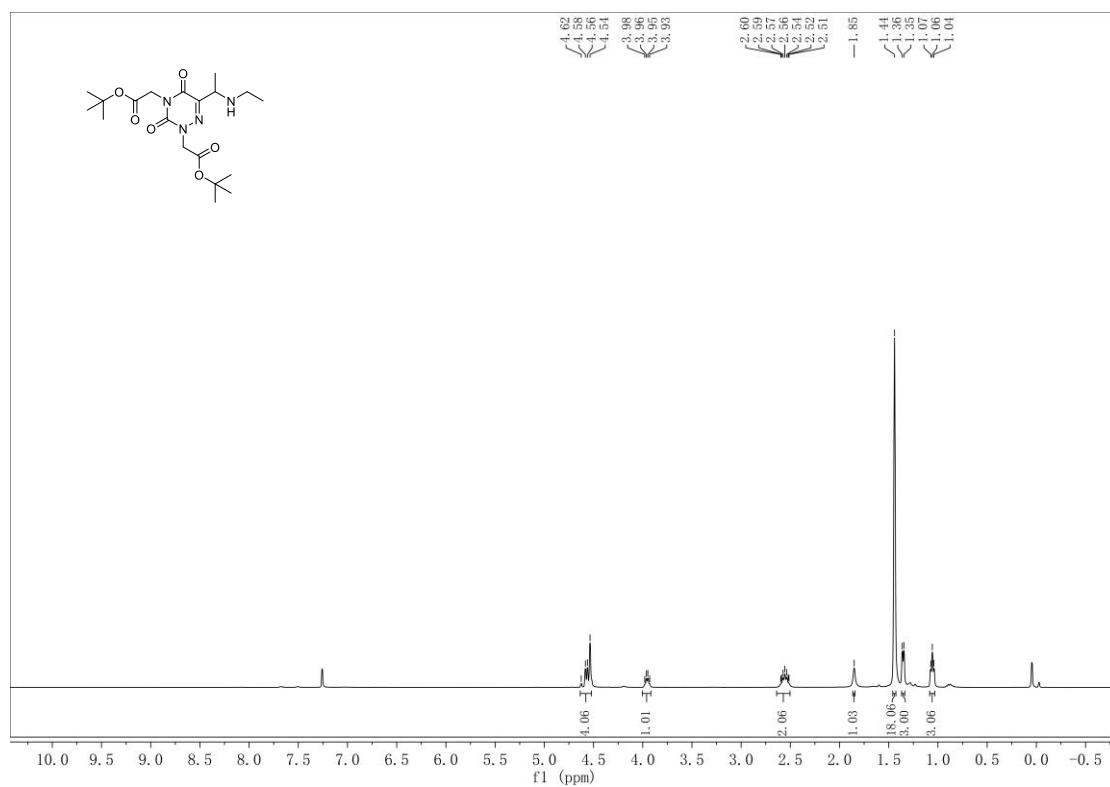


4k-¹³C

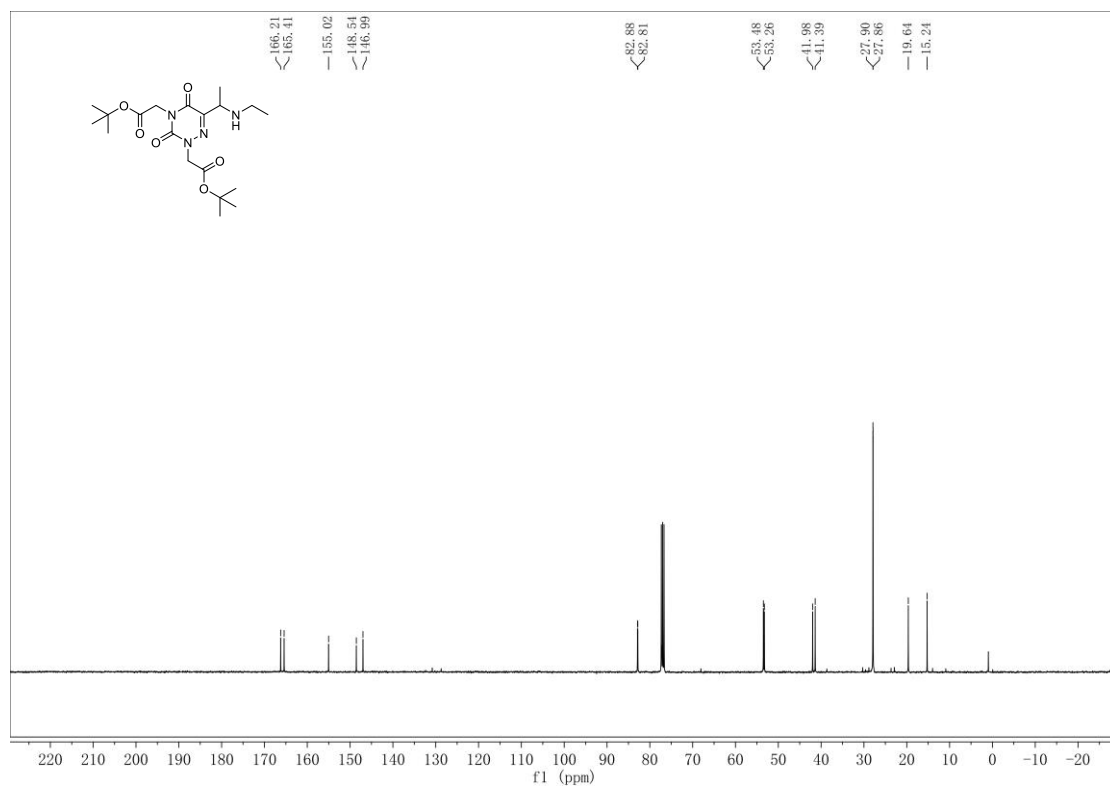


4I-¹H**4I-¹³C**

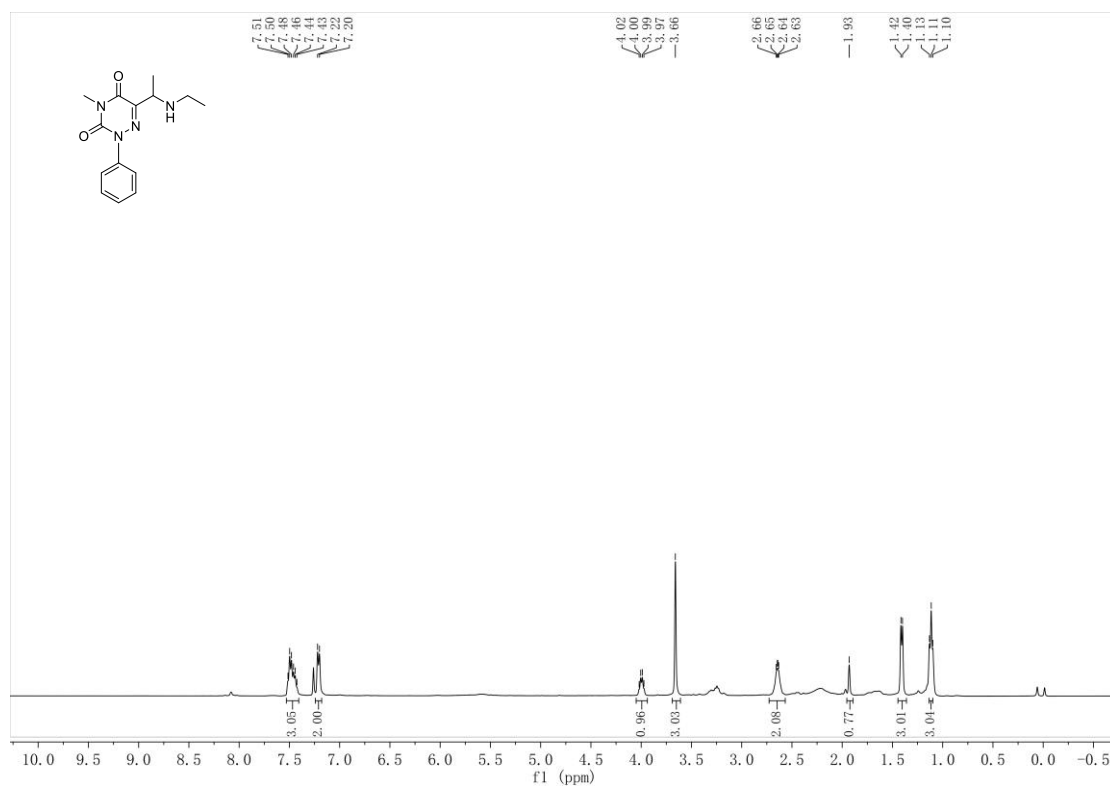
4m-¹H



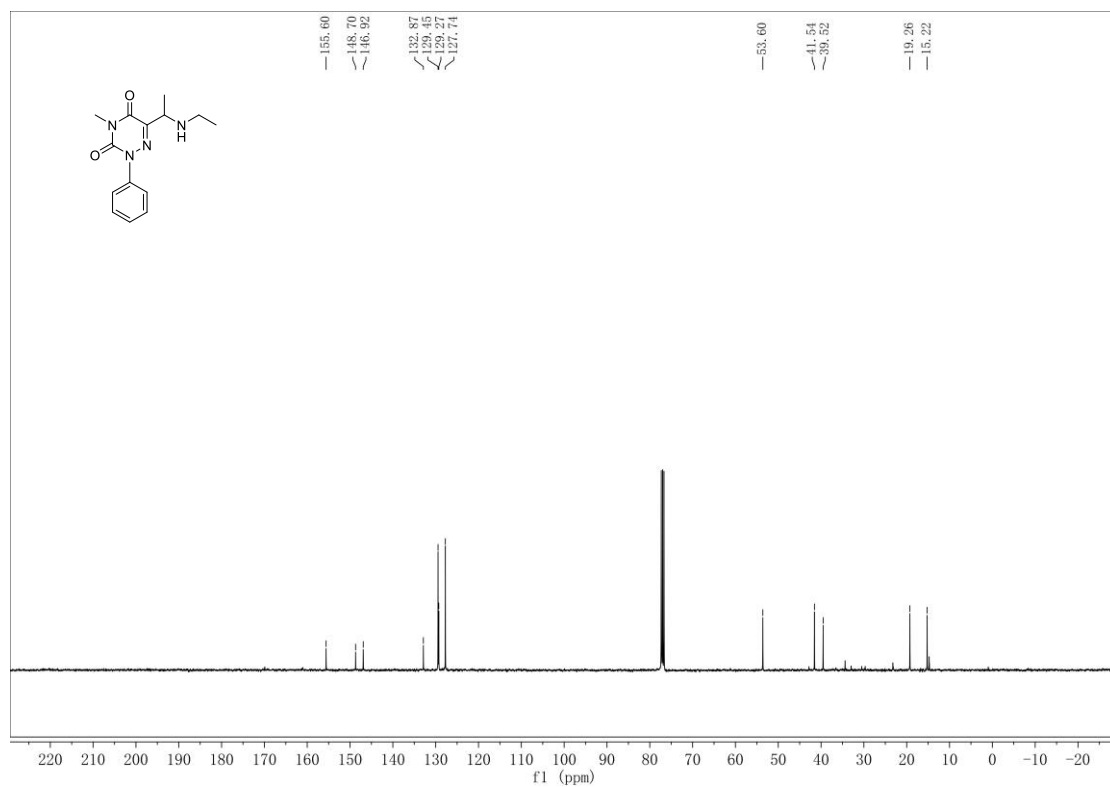
4m-¹³C



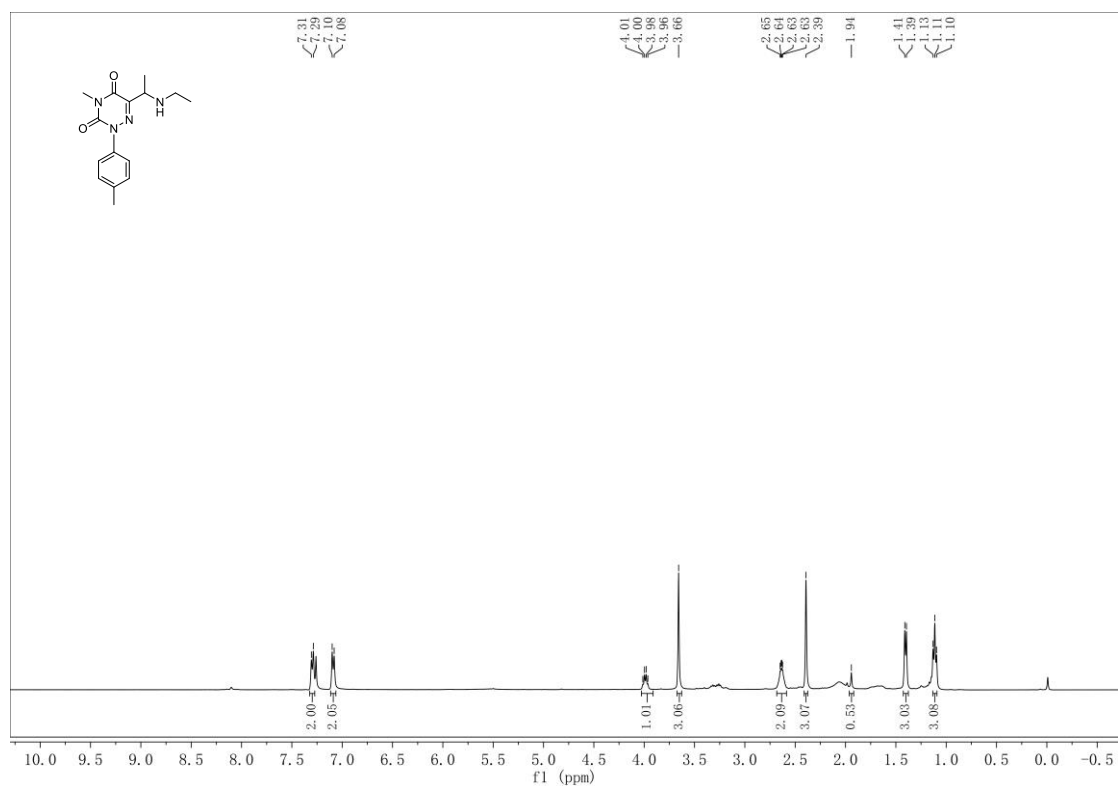
4n-¹H



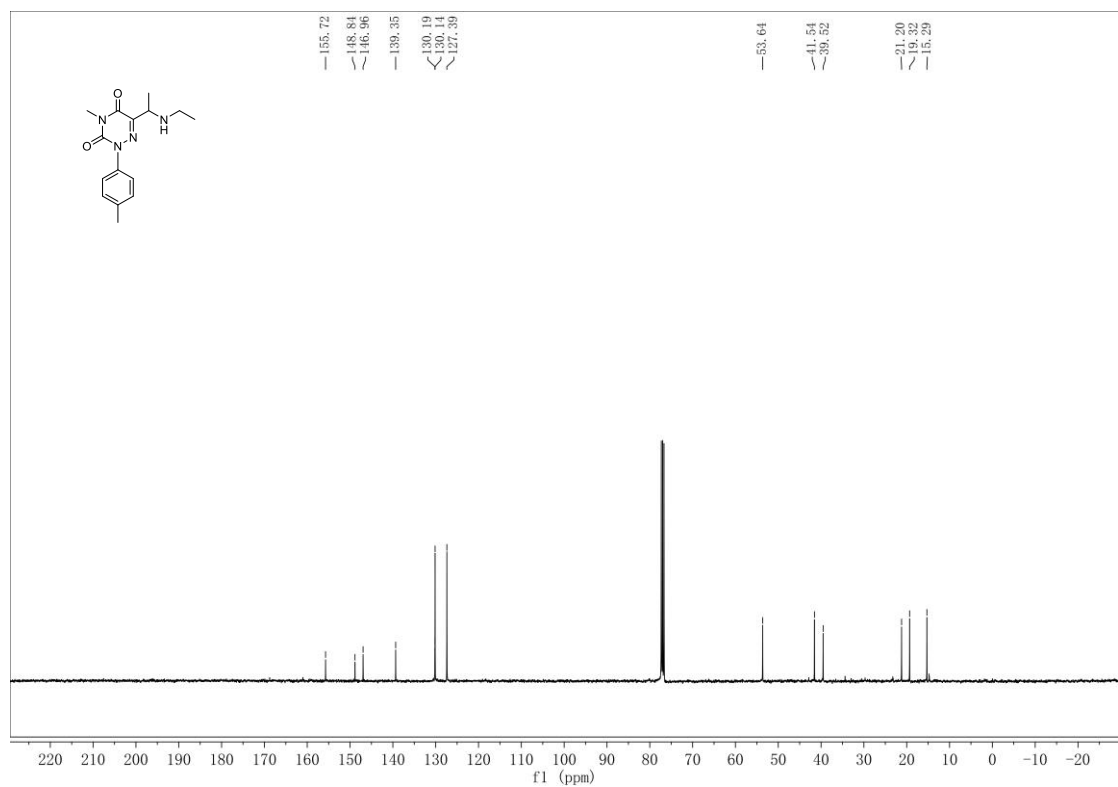
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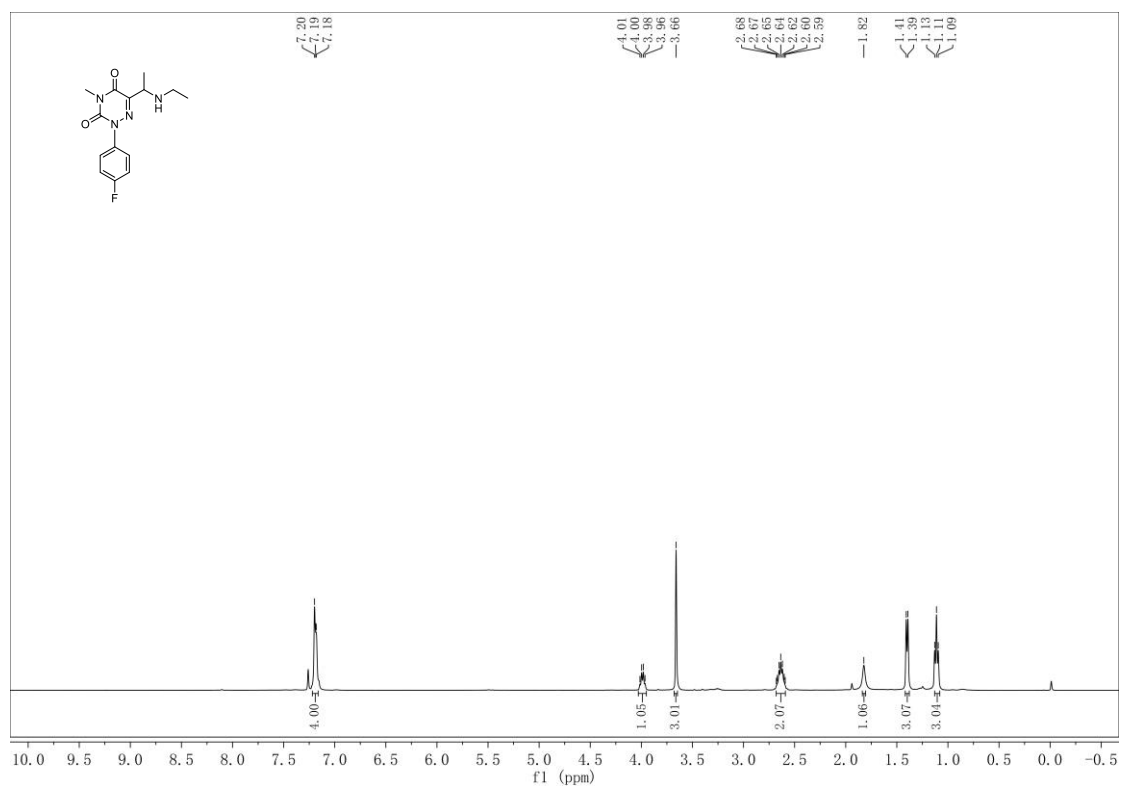
40-¹H



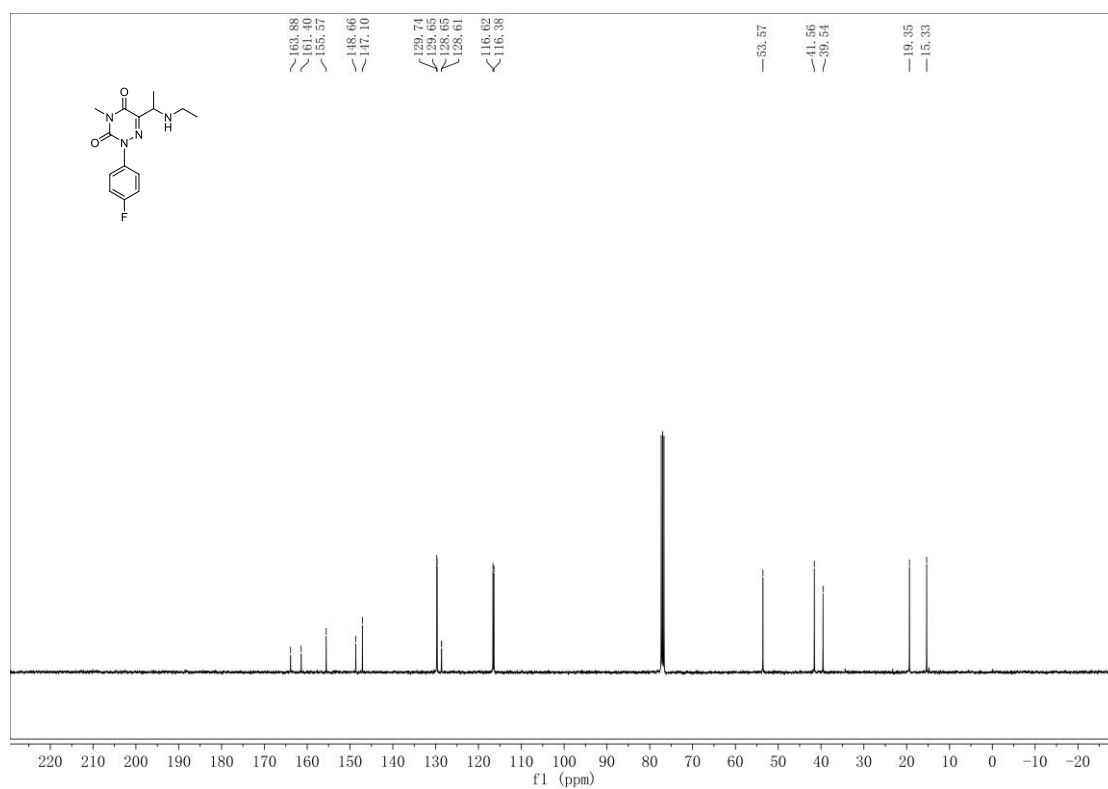
40-¹³C



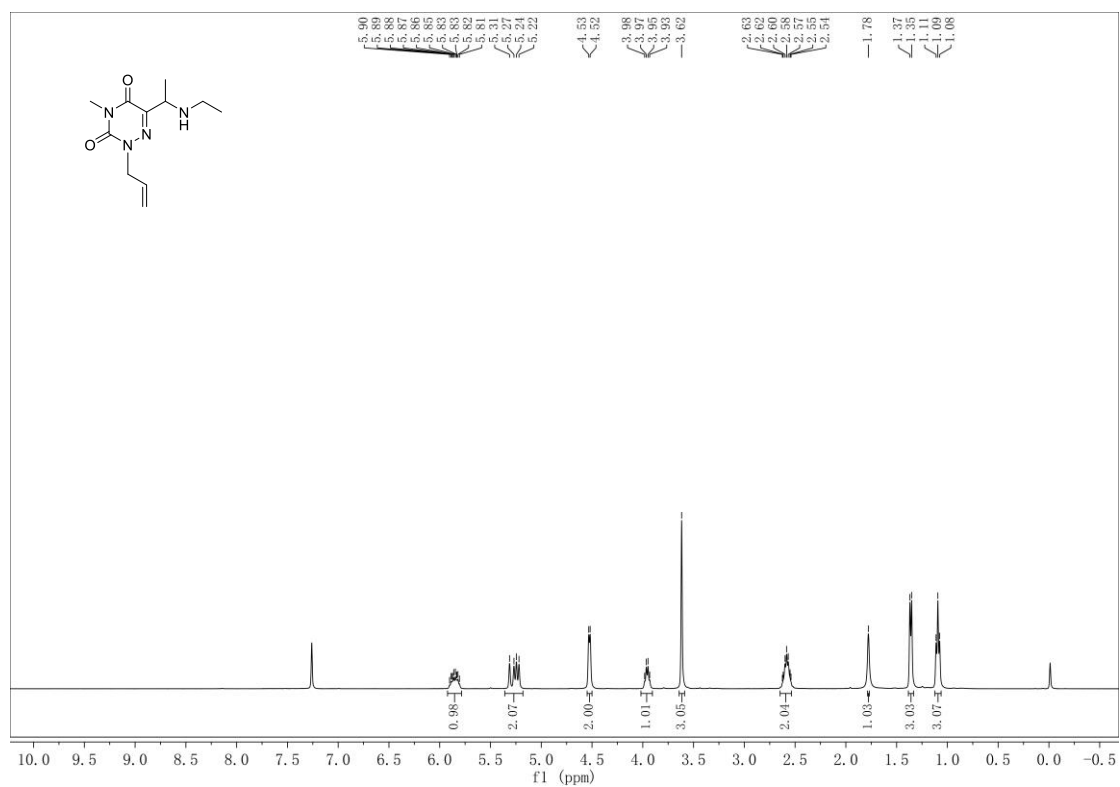
4p-¹H



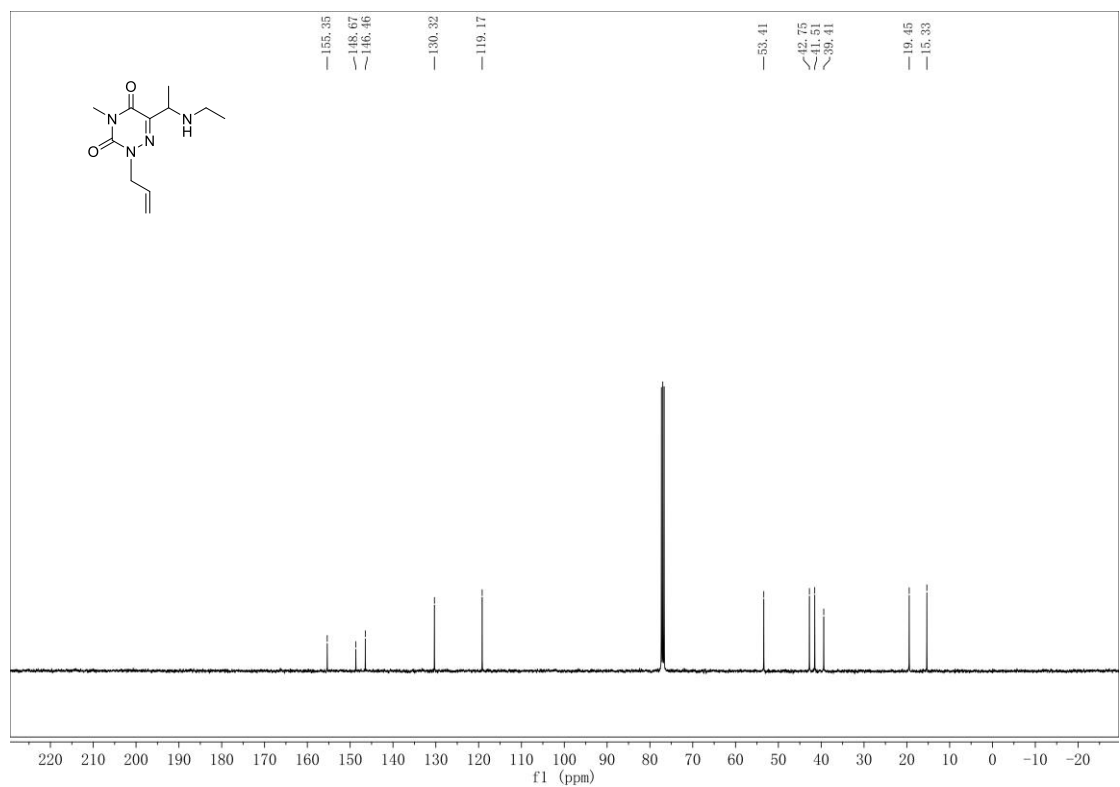
4p-¹³C



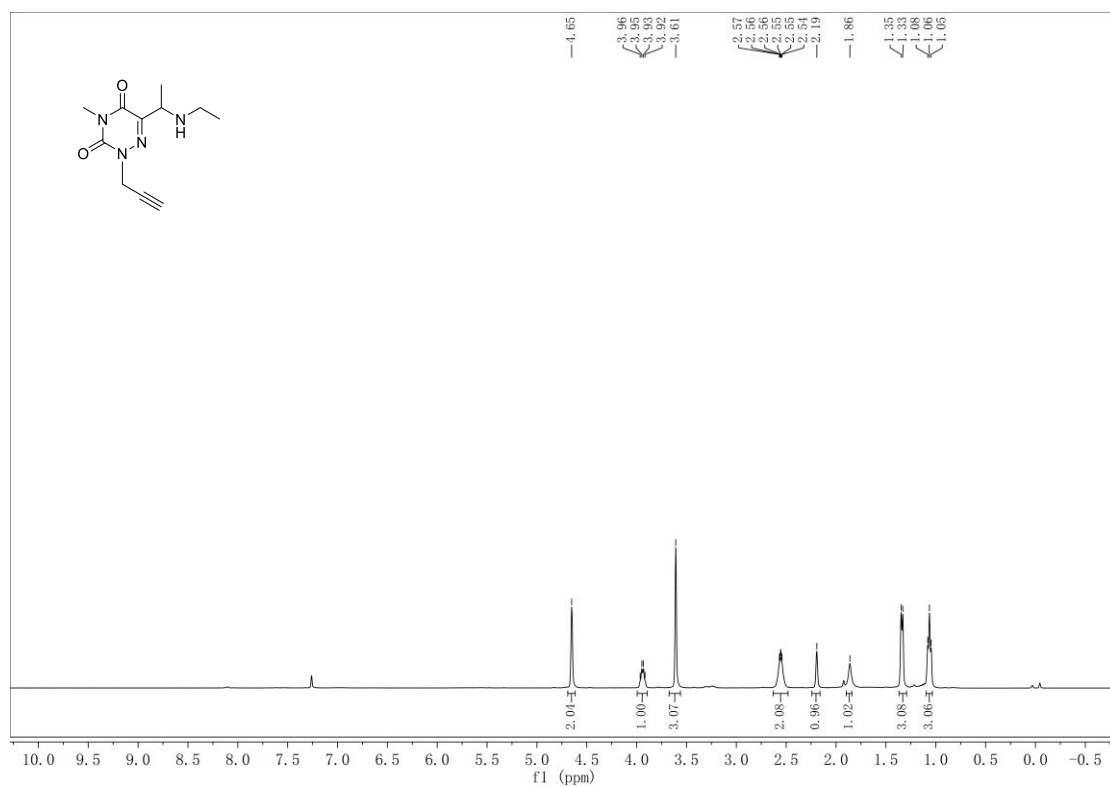
4q-¹H



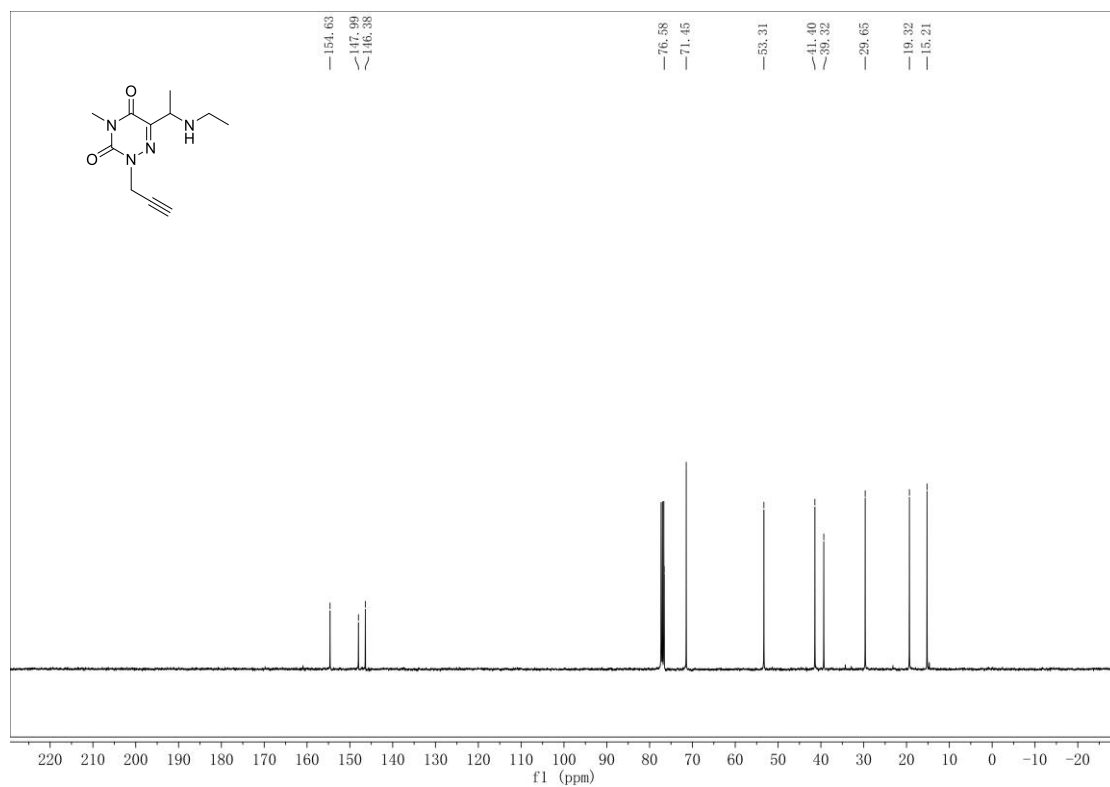
4q-¹³C



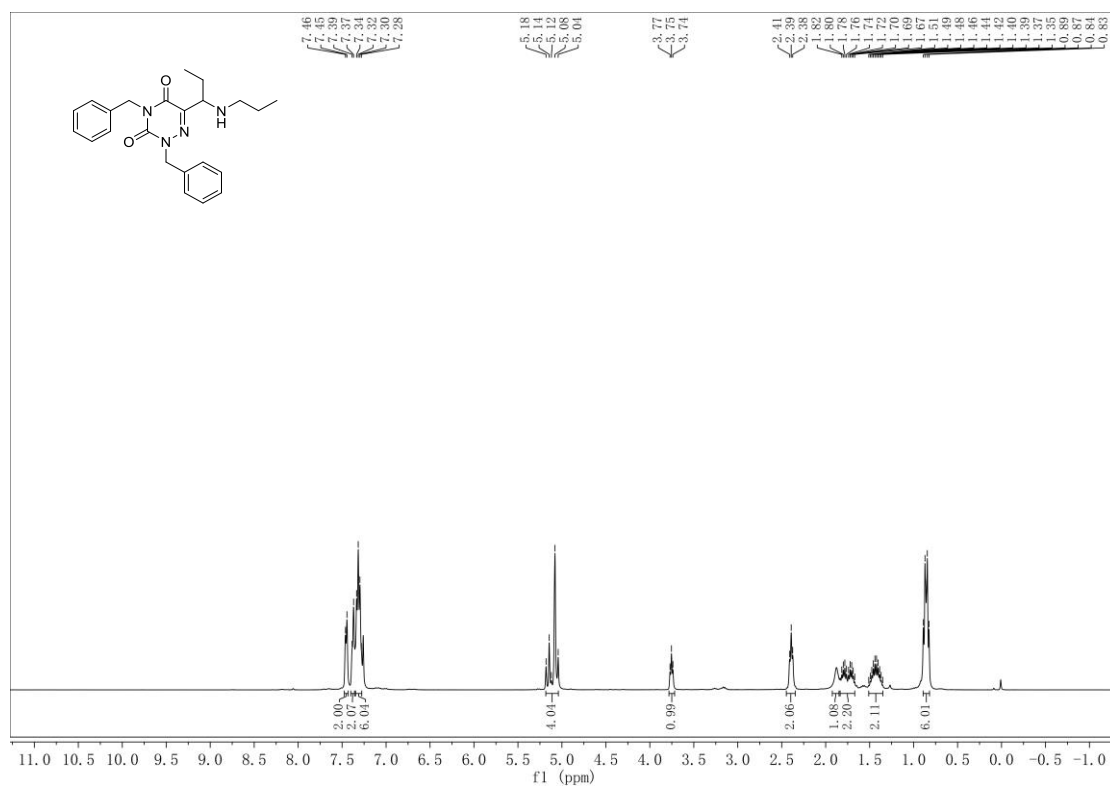
4r-¹H



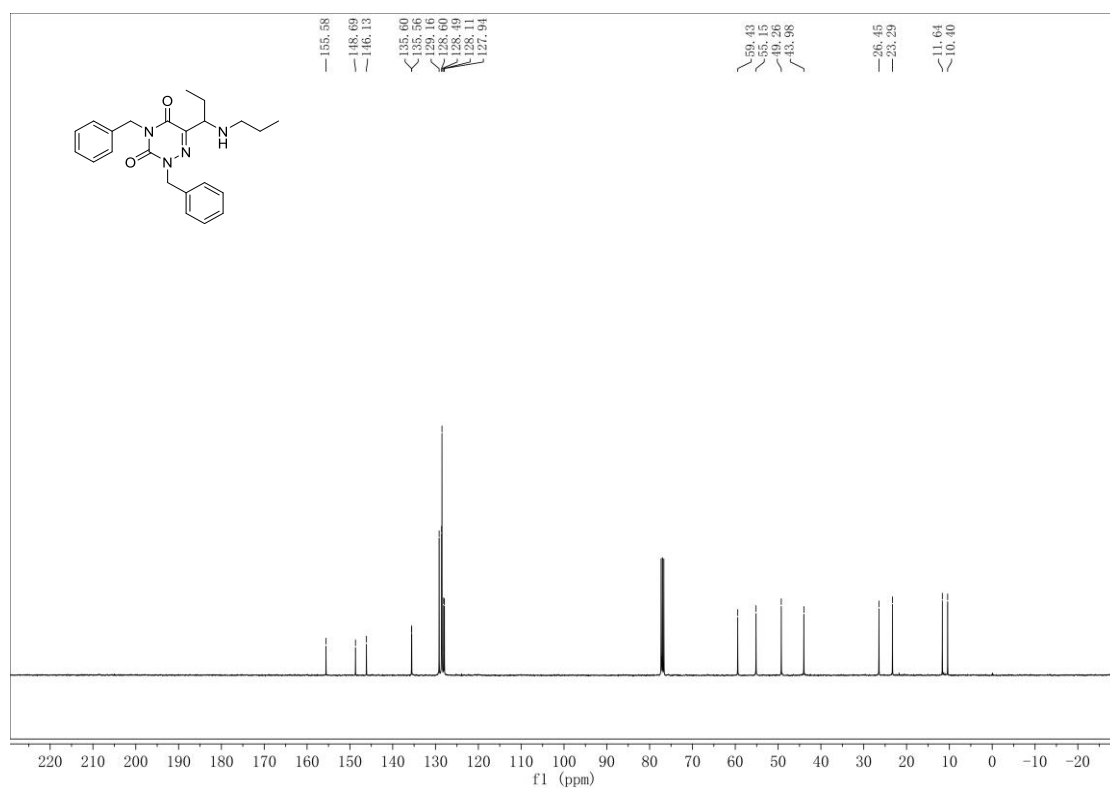
4r-¹³C



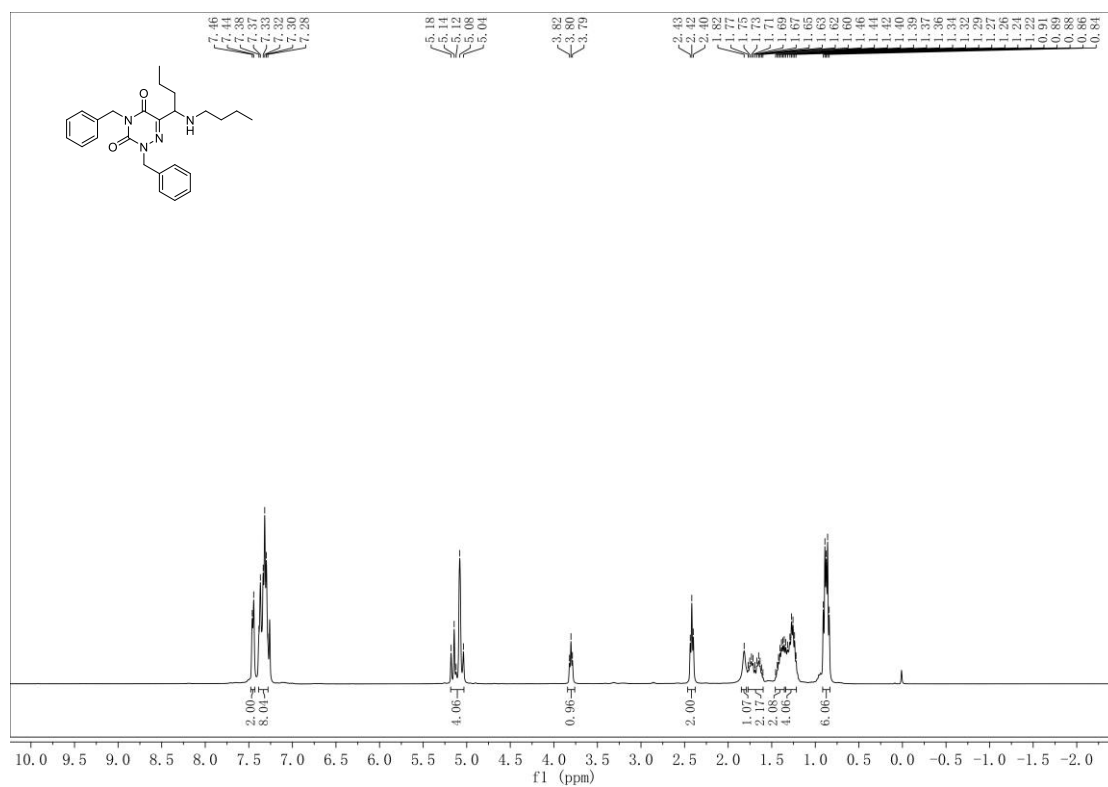
4s-¹H



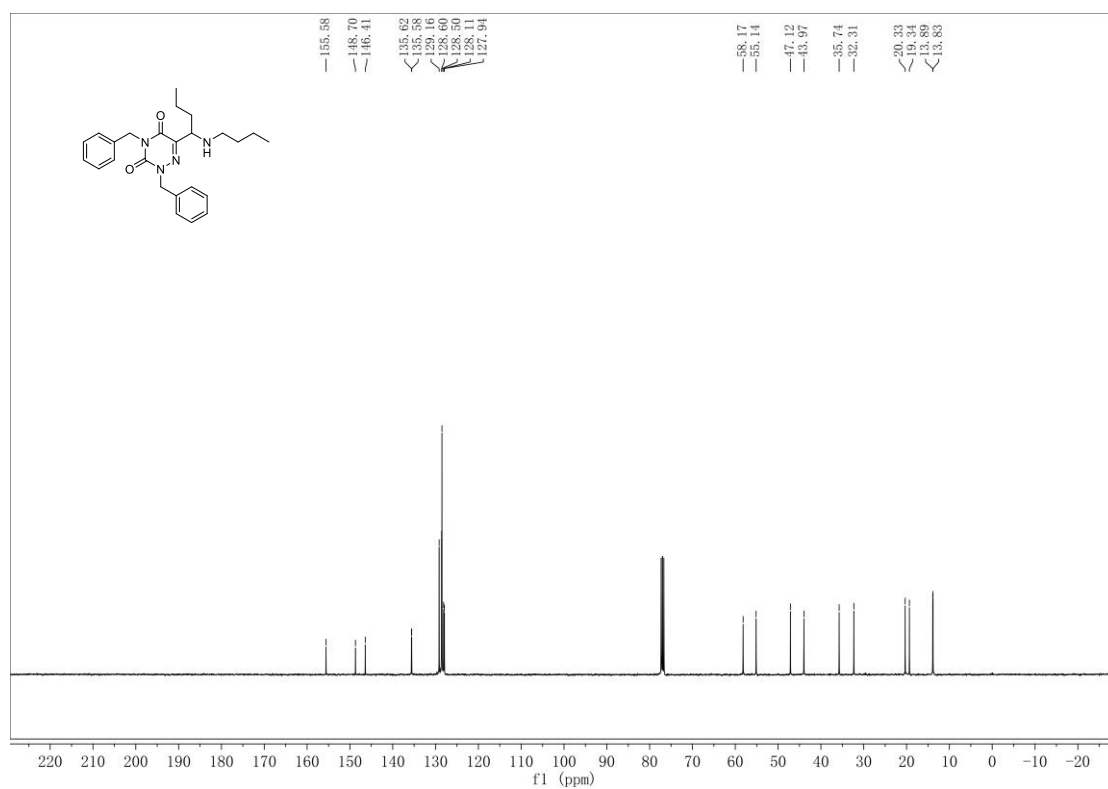
4s-¹³C



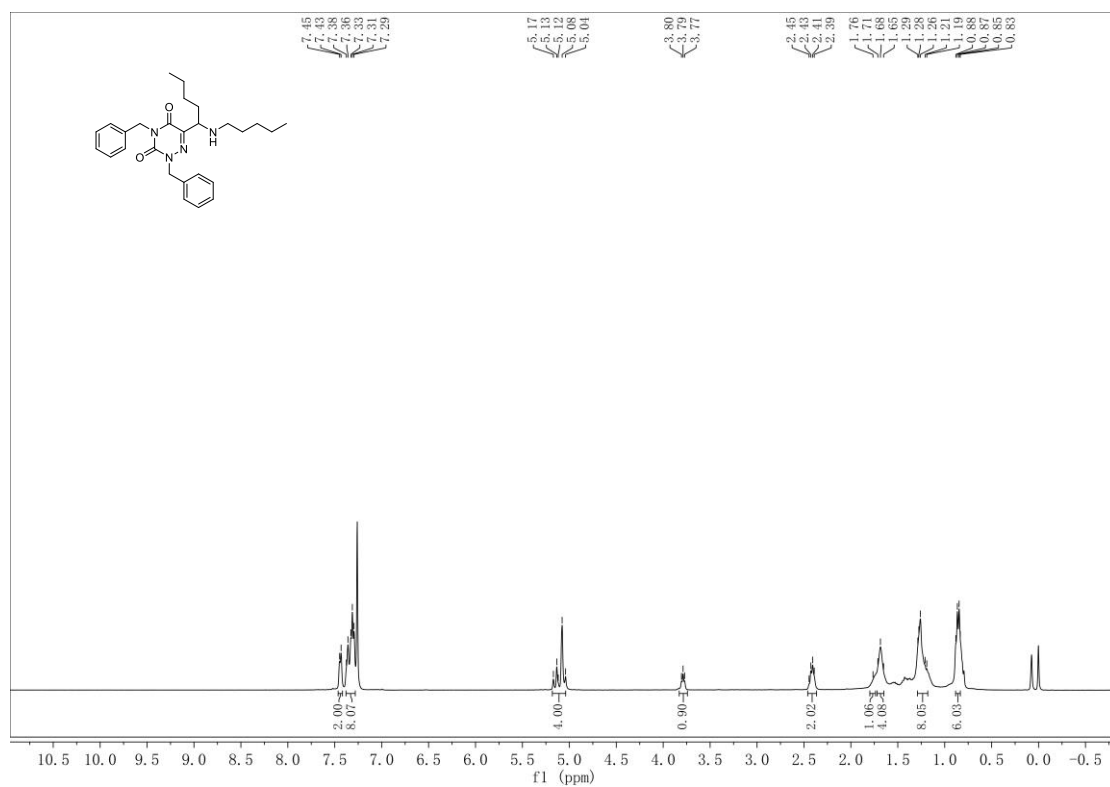
4t-¹H



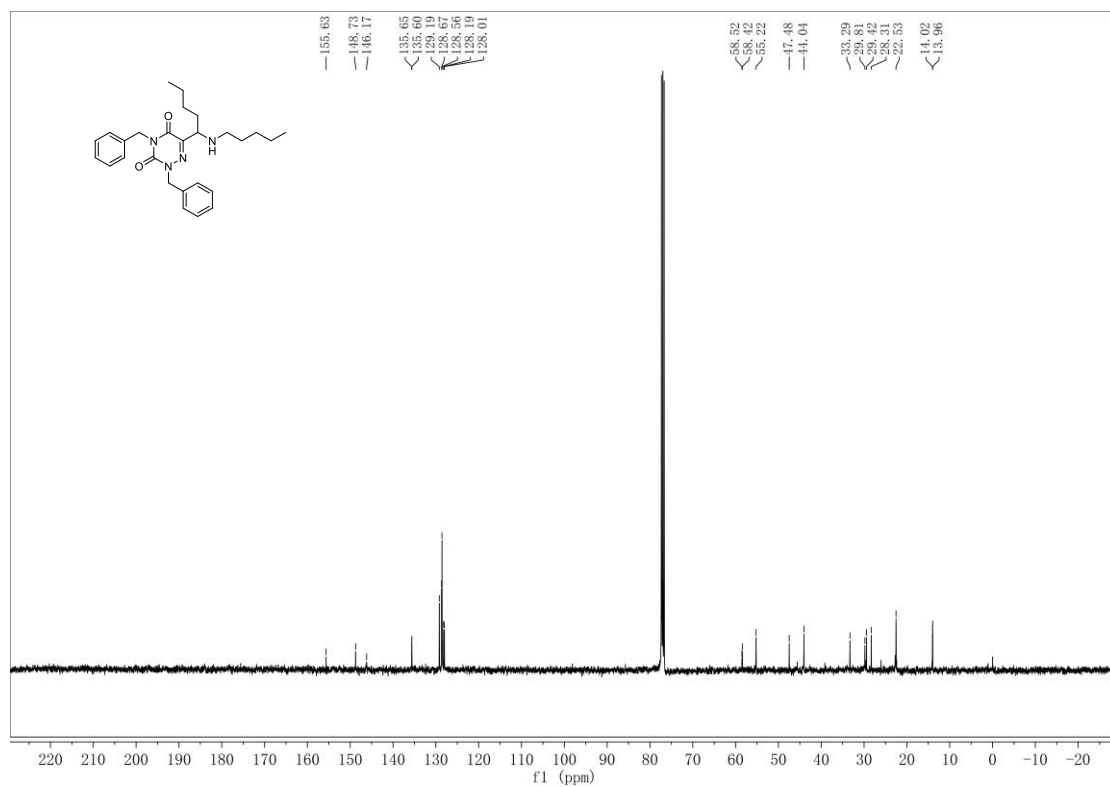
4t-¹³C



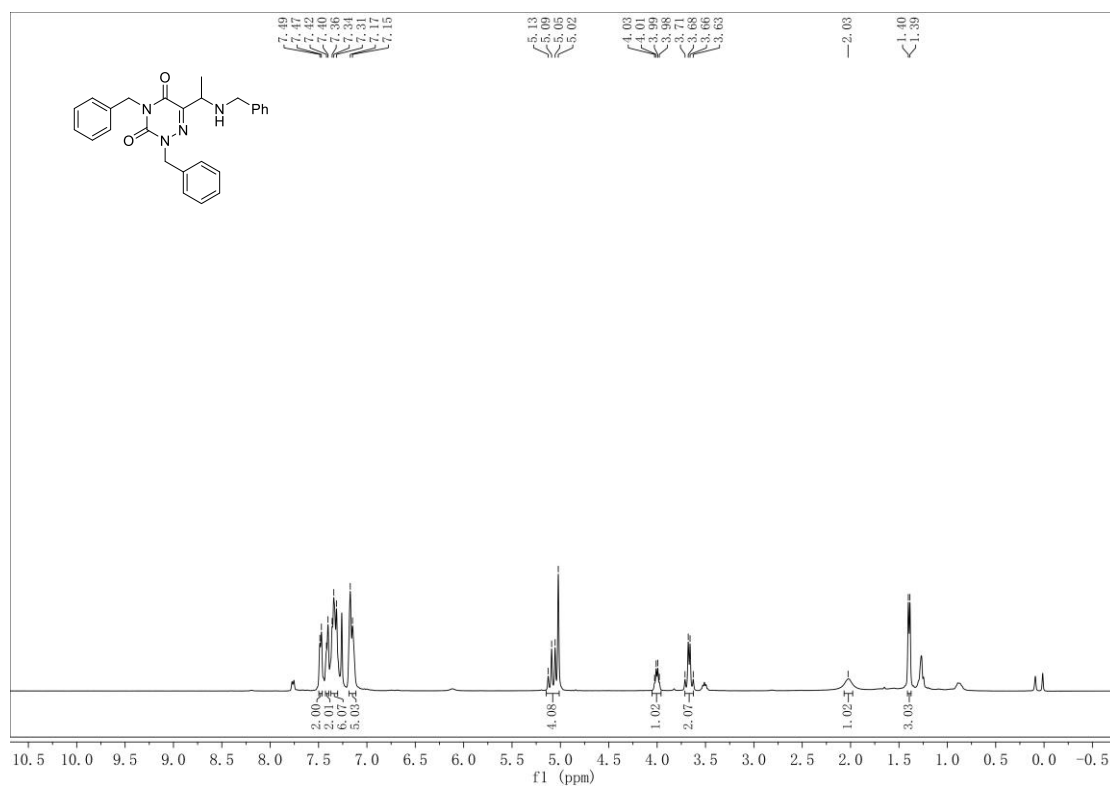
4u-¹H



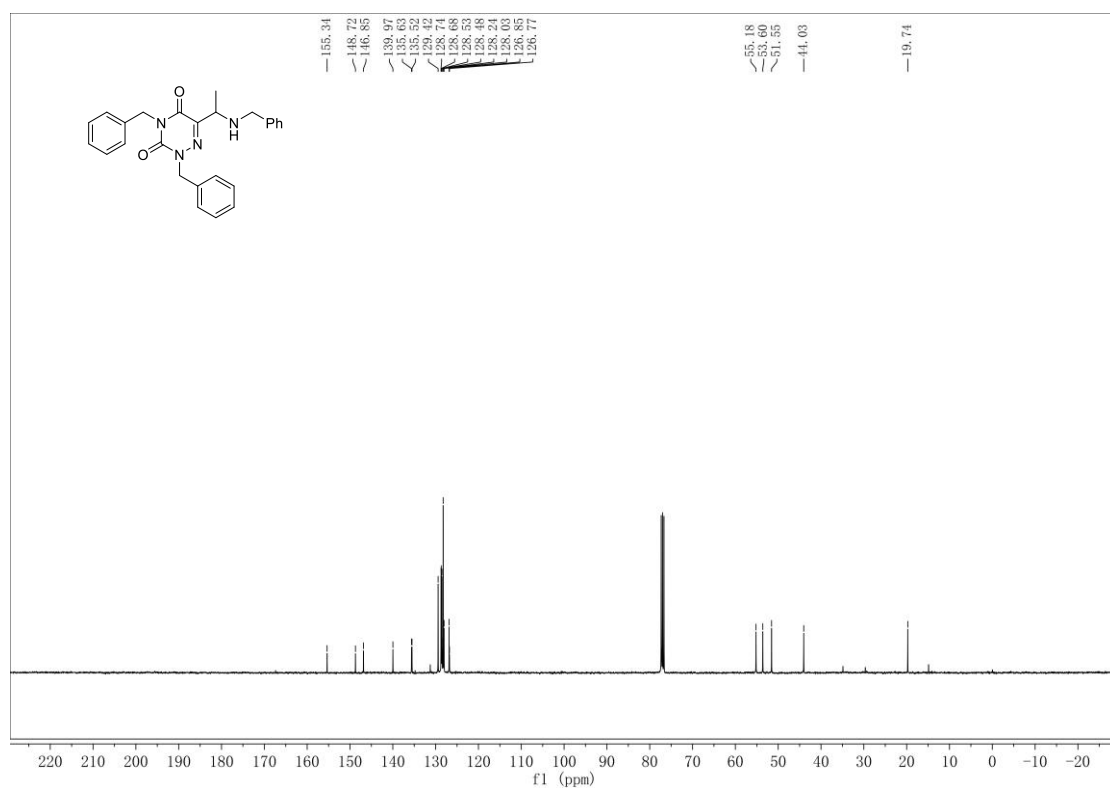
4u-¹³C



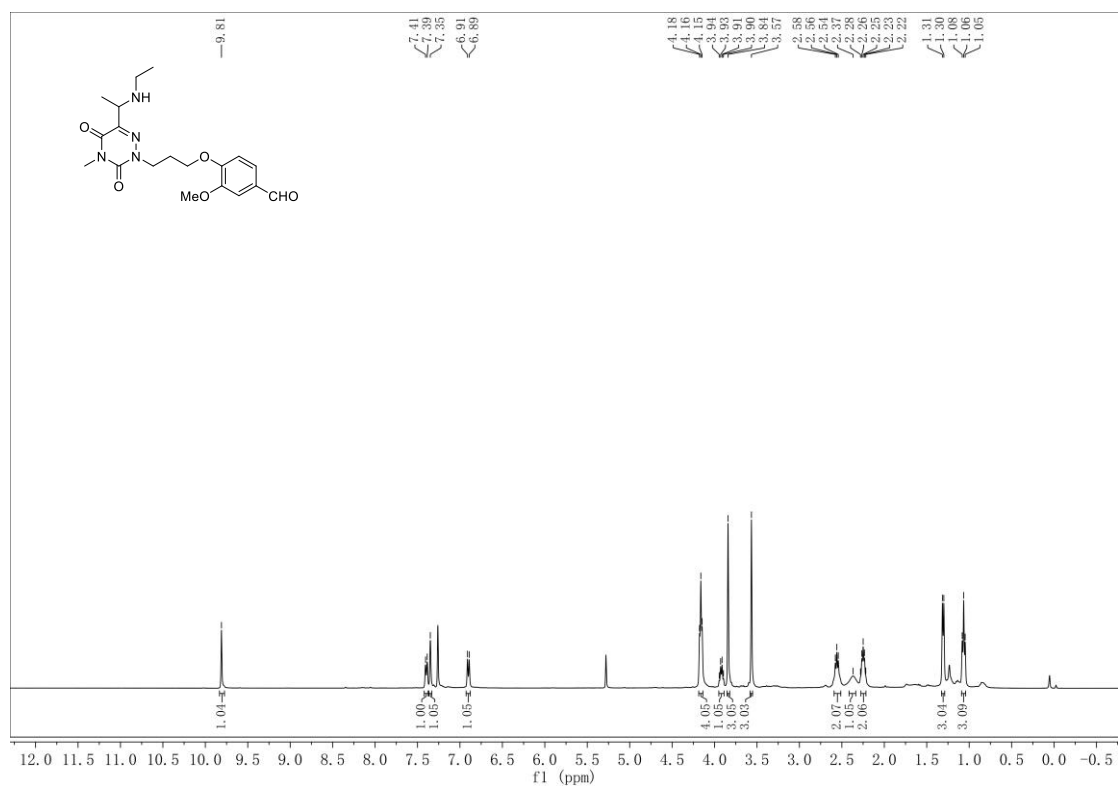
4v-¹H



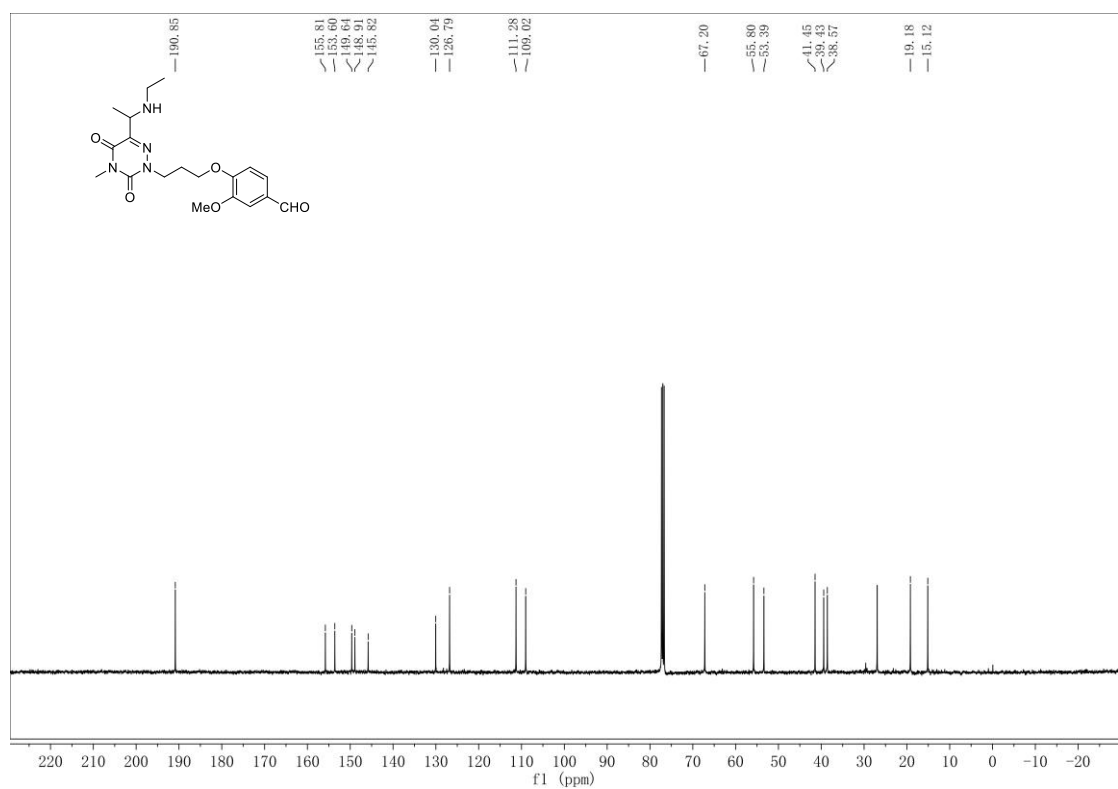
4v-¹³C



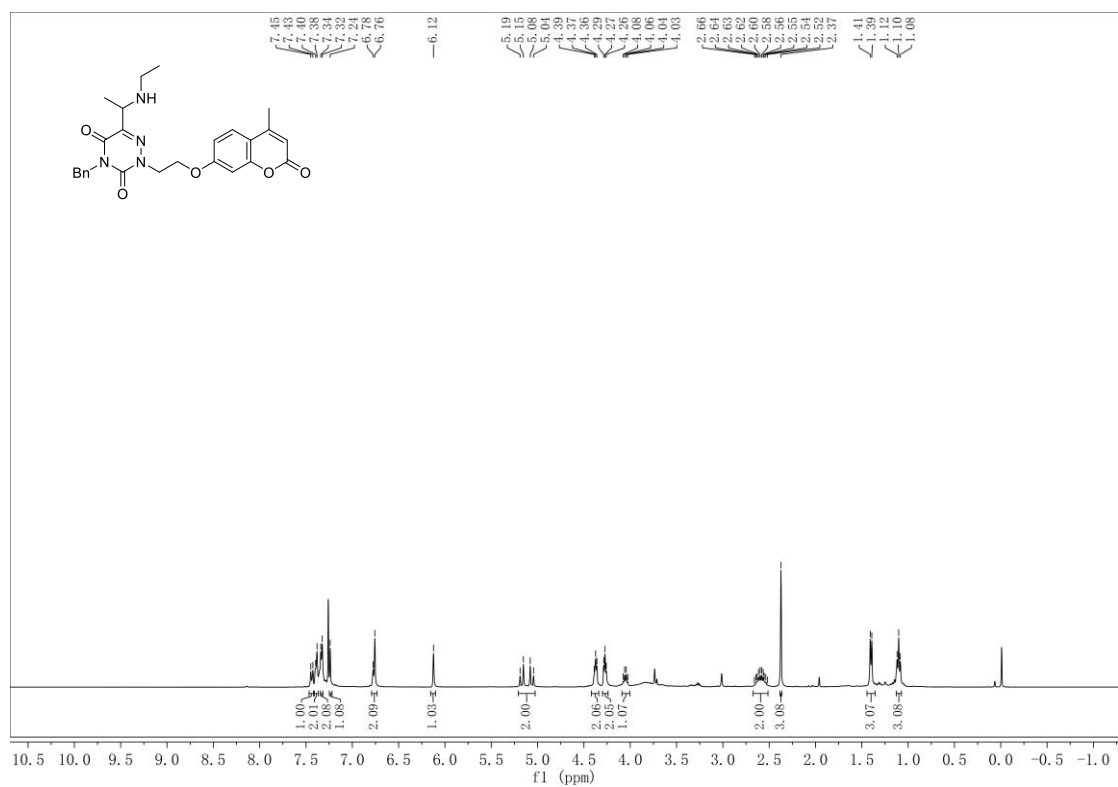
4w-¹H



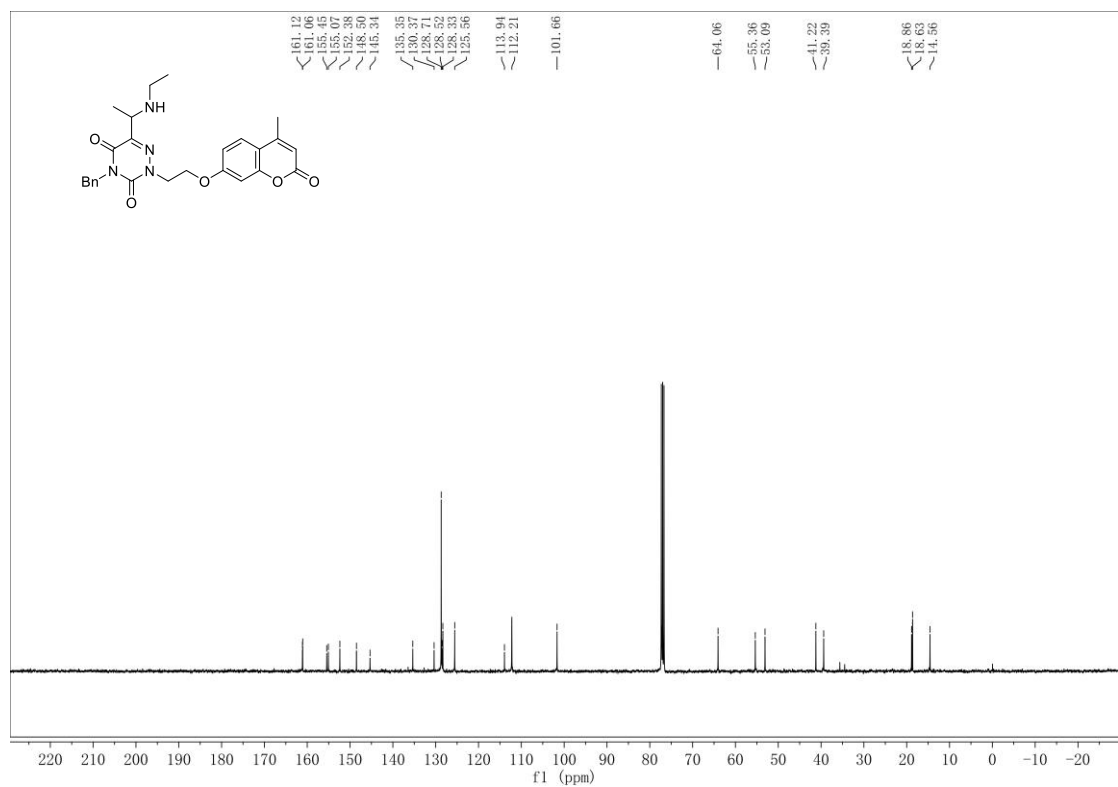
4w-¹³C



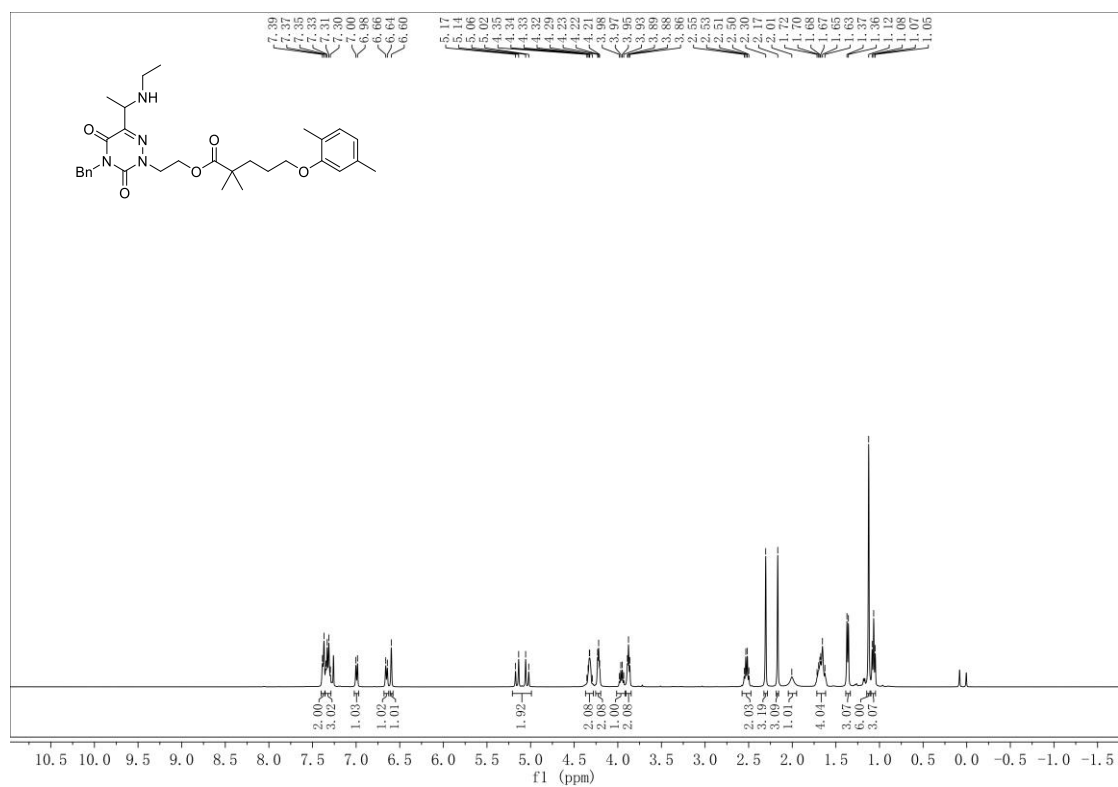
4x-¹H



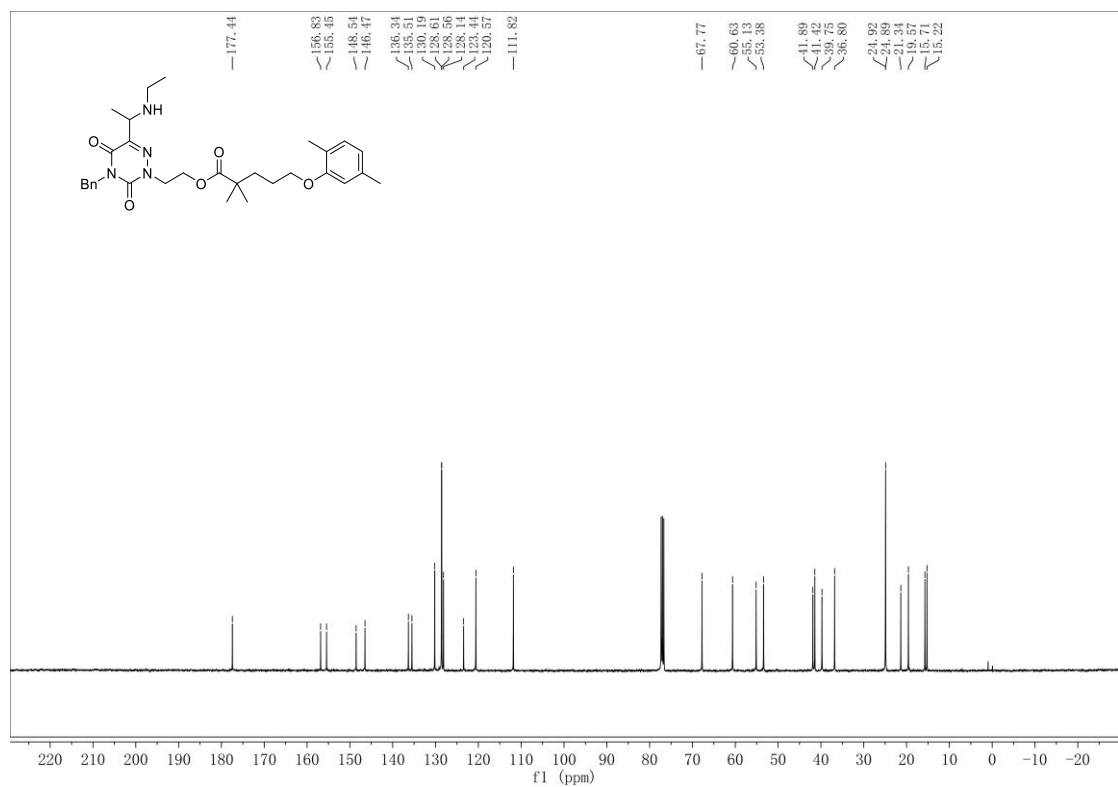
4x-¹³C



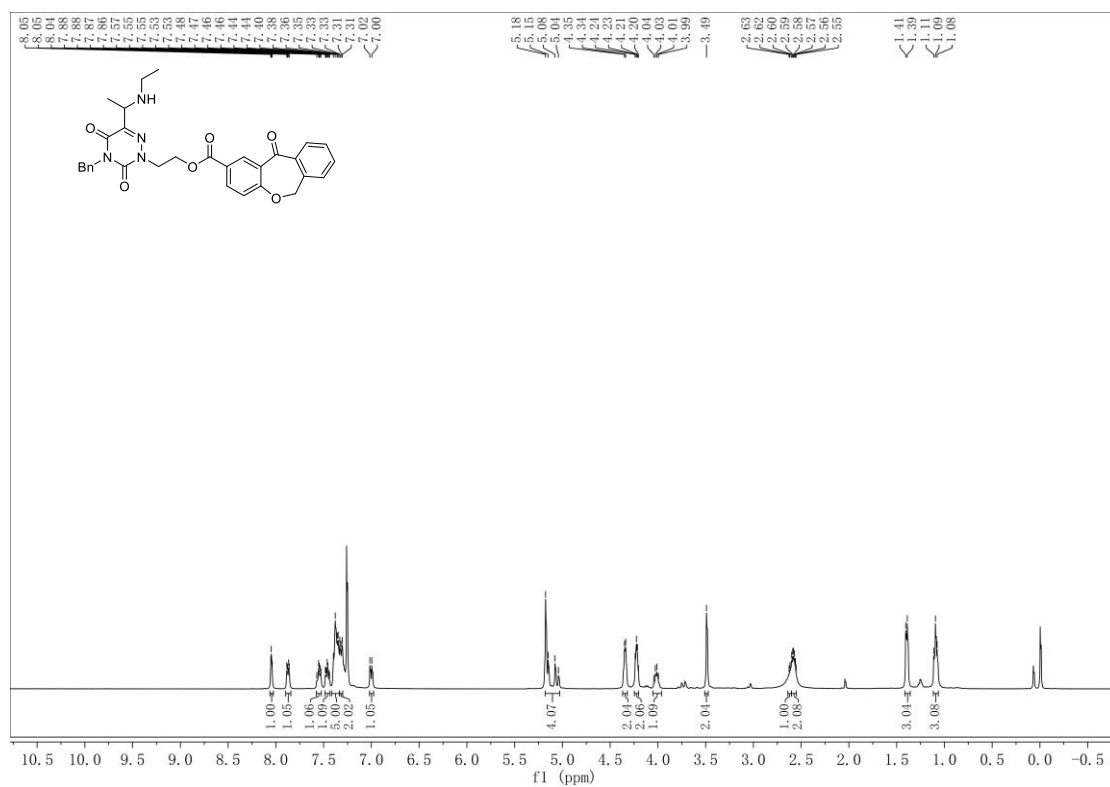
4y-¹H



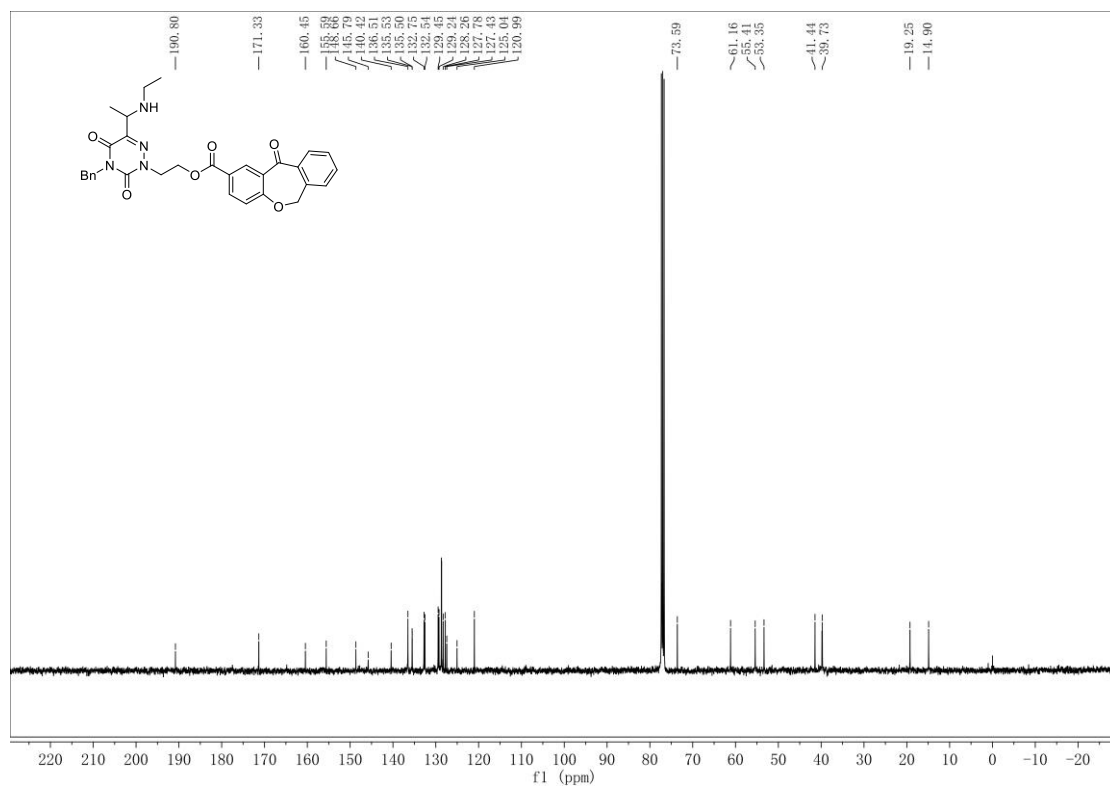
4y-¹³C



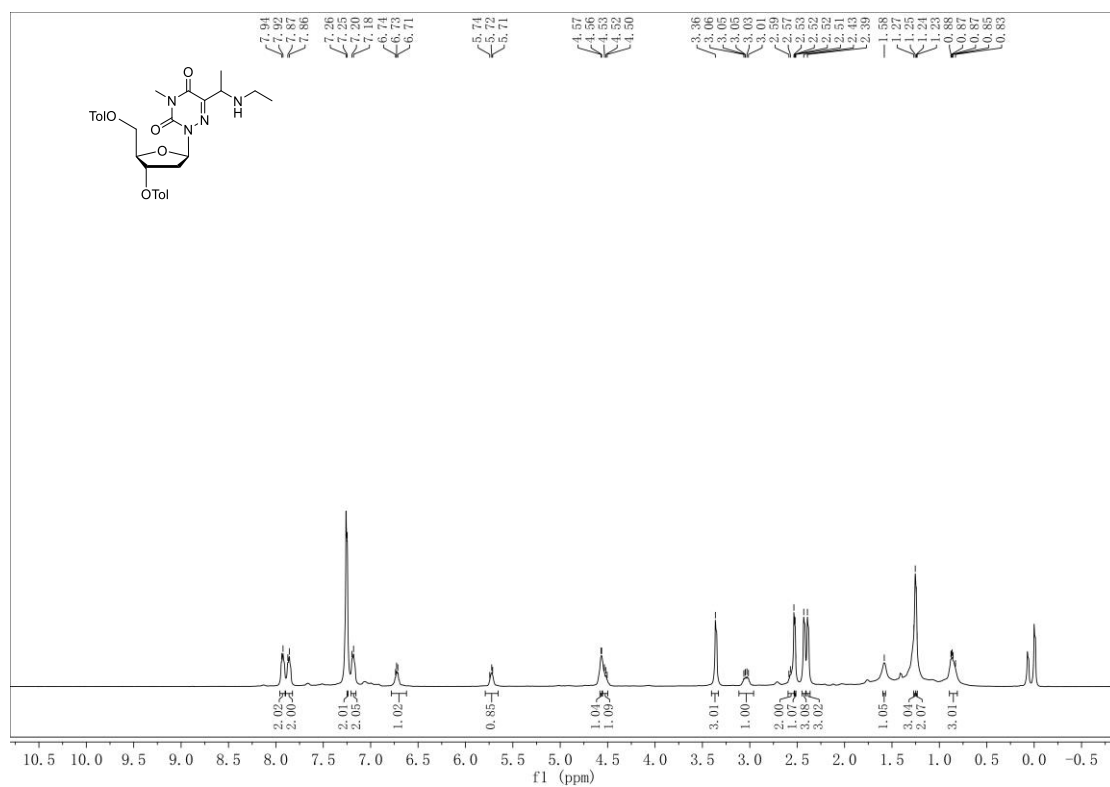
4z-¹H



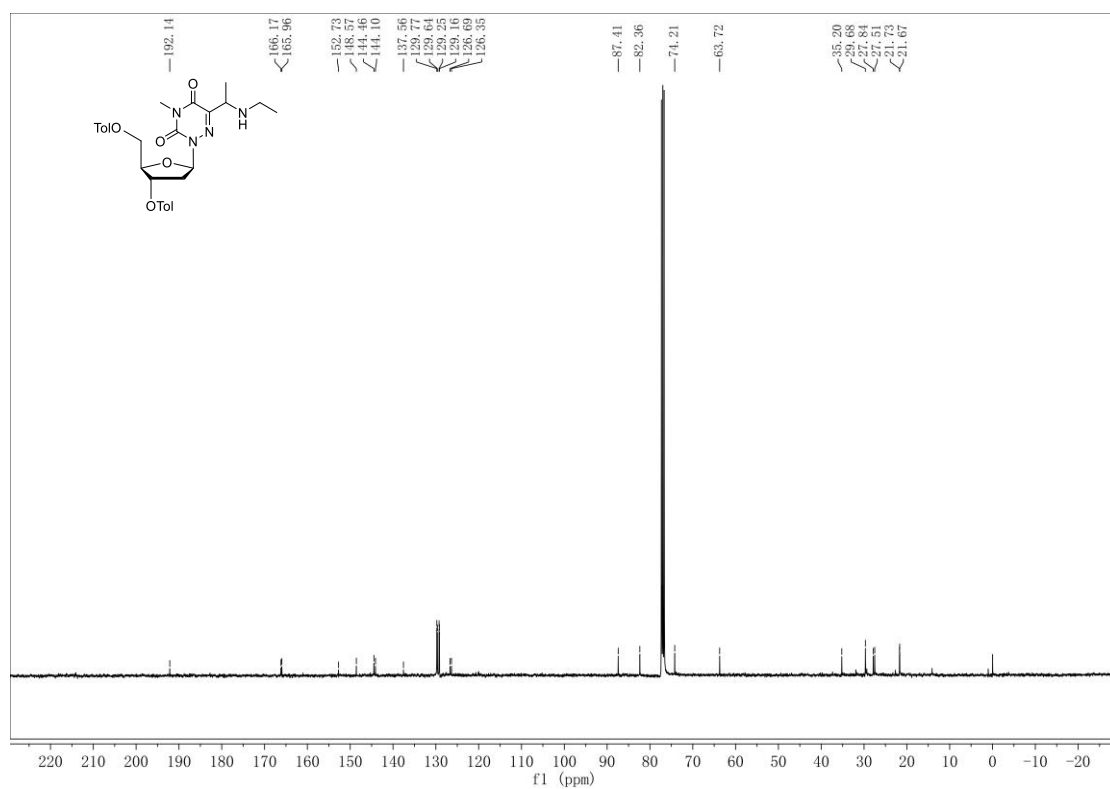
4z-¹³C



4aa-¹H



4aa-¹³C



XI. Computational details

Quantum chemistry calculations were conducted with the Gaussian 09 software package³. The structures were optimized by the density functional theory (DFT)⁴ with B3LYP-D3 functional^{5,6} with basis set def2-SVP⁷ using IEFPCM⁸ continuum solvent model (solvent = dichloroethane). Frequency analyses were performed at the same level of theory to verify the stationary points to be real minima or saddle points and to obtain the thermodynamic energy corrections at 298.15K. All transition states were confirmed by intrinsic reaction coordinate (IRC) calculations were performed to confirm the connection between two correct minima for a transition state. In order to get more accurate electronic energies, the single point energy were calculated at the M062x⁹-D3 /def2-TZVP level of theory using SMD¹⁰ continuum solvent model (solvent = dichloroethane) .

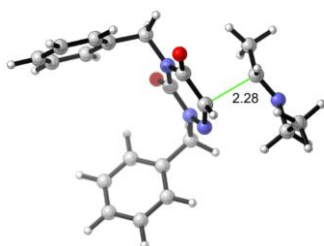
Table S3 Calculated energy data and imaginary frequencies for all structure.

	Energy (au)	Thermal correction to Enthalpy (au)	Thermal correction to Gibbs Free Energy (au)	Imaginary frequency (cm ⁻¹)
	M062x-D3 /def2TZVP/SMD	B3LYP-D3 /def2SVP/IEFPCM	B3LYP-D3 /def2SVP/IEFPCM	B3LYP-D3 / /def2SVP/IEFPCM
Substrate	-971.556072	0.312958	0.245328	None
HNEt₂	-213.767052	0.156382	0.118596	None
HNEt₂-CR	-213.557019	0.155963	0.116847	None
H₂NEt₂	-214.229553	0.172429	0.133913	None
NEt₂-C-Radical	-213.115582	0.142572	0.103719	None
NEt₂-N-Radical	-213.110557	0.141358	0.101454	None
³O₂	-150.327196	0.007176	-0.016086	None
¹O₂	-150.26844	0.00714	-0.015087	None
HO₂	-150.914738	0.017938	-0.008023	None
TS-1	-1184.681484	0.457714	0.371104	-178.06
INT-1	-1184.699442	0.459995	0.375301	None
4a	-1184.138656	0.44926	0.365307	None
H₂O₂	-151.557405	0.029554	0.003583	None
TS-2	-1184.649872	0.454957	0.371605	-1602.27
INT-1-pAcid	-1527.144544	0.540332	0.438578	None
TS-2-pAcid	-1527.130378	0.537035	0.440843	-1368.06
INT-2-pAcid	-1527.146218	0.541073	0.442392	None

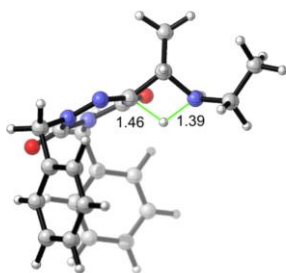
TS-3-pAcid	-1527.118126	0.53901	0.438666	-238.20
TS-3	-1184.681925	0.458861	0.374447	-369.96
NH₂Et	-135.15913	0.097525	0.066802	None
INT-3	-1049.53404	0.358385	0.283927	None

Structures of Transition states

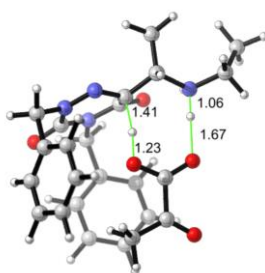
TS-1



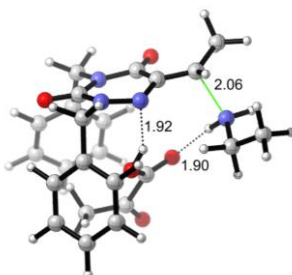
TS-2



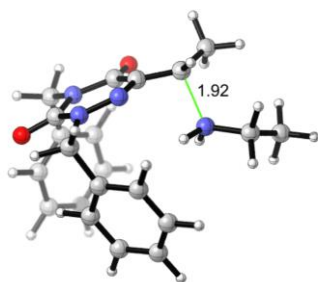
TS-2-pAcid



TS-3-pAcid



TS-3



Coordinations

Substrate

Charge = 0 Multiplicity = 1

C	0.14270500	-2.73659200	-1.15732100
C	0.01393000	-1.12079700	1.08142900
C	-1.18945300	-2.31375200	-0.70640200
N	-1.15944100	-1.51881200	0.44526100
N	1.18784500	-1.62555200	0.52033100
N	1.23976900	-2.39117400	-0.57409200
O	0.02279000	-0.39062100	2.05642000
O	-2.22868000	-2.61037500	-1.27100600
C	2.48522100	-1.18101500	1.06332200
H	2.34683600	-1.01827900	2.13837400
H	3.17940100	-2.01721700	0.91422100
C	-2.43379100	-0.99210900	0.97562600
H	-2.33405200	-0.94246200	2.06577200
H	-3.20274500	-1.72846500	0.71544700
C	-2.77210700	0.36758100	0.39920900
C	-2.39039600	1.54070900	1.06833800
C	-3.44052900	0.46736300	-0.83180900
C	-2.67966000	2.79403500	0.51956100
H	-1.85293200	1.46251100	2.01568400
C	-3.72807400	1.72060400	-1.38061900
H	-3.72341200	-0.44652900	-1.35922600
C	-3.34924600	2.88670900	-0.70559000
H	-2.38005900	3.70164900	1.05005400
H	-4.25114600	1.78755500	-2.33814400
H	-3.57571300	3.86649400	-1.13414300
C	2.98208500	0.07454000	0.37976700
C	3.84507900	-0.01338300	-0.72243900
C	2.54339600	1.33847400	0.80711200
C	4.27020000	1.14286500	-1.38462600
H	4.18556700	-0.99454400	-1.06401400
C	2.96650100	2.49401900	0.14424500
H	1.85946600	1.40637700	1.65597300
C	3.83138900	2.39890800	-0.95224400

H	4.94625300	1.06257600	-2.23973500
H	2.62072600	3.47323100	0.48538500
H	4.16385500	3.30319000	-1.46845200
H	0.20436800	-3.36832200	-2.04635900

HNEt₂

Charge = 0 Multiplicity = 1

N	-0.07487000	-0.67659600	0.20331600
H	-0.10553000	-0.66698800	1.22414800
C	1.31181800	-0.61543700	-0.24474200
C	2.11492200	0.62396500	0.17536900
H	1.31583800	-0.69647100	-1.34728600
H	1.82616700	-1.51902000	0.12763100
H	3.15911800	0.55018000	-0.17078800
H	1.69003200	1.55005200	-0.24352100
H	2.12963900	0.72597000	1.27412900
C	-0.96116600	0.35632900	-0.31874300
C	-2.40120300	0.11965400	0.12641600
H	-0.90475900	0.32264100	-1.42236100
H	-0.66071600	1.38895700	-0.03328300
H	-3.07808900	0.87807000	-0.29802400
H	-2.74631600	-0.87788100	-0.18903600
H	-2.48751900	0.17359200	1.22537900

HNEt₂-CR

Charge = 1 Multiplicity = 2

N	-0.00411400	-0.39358000	0.44142400
H	-0.16490600	-0.22090500	1.44146300
C	1.34803200	-0.61547600	0.01165500
C	2.10083700	0.73301200	-0.10498400
H	1.32470900	-1.13058400	-0.95902100
H	1.84177000	-1.25224400	0.76286300
H	3.12670000	0.51219300	-0.43283400
H	1.61664300	1.38214600	-0.84826200
H	2.13913200	1.24969200	0.86433300
C	-1.13731500	-0.34788000	-0.43731500
C	-2.28912100	0.48902000	0.09987600
H	-1.45012500	-1.40848400	-0.57890300
H	-0.78090000	-0.01862500	-1.42888100
H	-3.13062000	0.43062600	-0.60408400
H	-2.63557300	0.11591600	1.07584200
H	-1.99263100	1.54327300	0.20212700

H₂NEt₂

Charge = 1 Multiplicity = 1

N	0.04863800	0.64911200	0.22513700
H	0.41612500	1.58963900	0.02777700
C	-1.38579200	0.59013800	-0.24831200
C	-2.09578700	-0.68241700	0.17699300
H	-1.35460800	0.70131900	-1.34141600
H	-1.87549900	1.47914800	0.17235100
H	-3.14862000	-0.61141800	-0.13212300
H	-1.67123500	-1.57969200	-0.29507600
H	-2.07567600	-0.80982500	1.27074400
C	0.98794600	-0.37089800	-0.36690500
C	2.40469100	-0.17718500	0.14321700
H	0.92127200	-0.25577600	-1.45768100
H	0.59405600	-1.35929900	-0.09921500
H	3.05043000	-0.94980400	-0.29810000
H	2.81063200	0.80534100	-0.14321900
H	2.45722700	-0.27920100	1.23847800
H	0.06908300	0.56795800	1.25155900

NEt₂-C-Radical

Charge = 0 Multiplicity = 2

N	0.07190700	-0.61692800	-0.24108000
C	-1.31836700	-0.59997500	0.18764300
C	-2.07389100	0.69305800	-0.13819100
H	-1.33645800	-0.77607200	1.27754900
H	-1.83143800	-1.46075100	-0.27403100
H	-3.11240900	0.64856400	0.22869200
H	-1.57552600	1.55766100	0.32838000
H	-2.10383800	0.86575500	-1.22713600
C	1.01004600	0.17675000	0.41847500
C	2.39535300	0.24364000	-0.13718400
H	0.86651500	0.23680200	1.50453600
H	3.00244500	0.98308100	0.40808400
H	2.93689400	-0.72751600	-0.08522100
H	2.39235100	0.53923800	-1.20350800
H	0.17927400	-0.62910500	-1.25424900

NEt₂-N-Radical

Charge = 0 Multiplicity = 2

N	0.00000600	0.30498000	0.00008400
C	1.20350800	-0.48025400	0.01192400
C	2.45999500	0.38508300	-0.00551200
H	1.20558900	-1.18170700	-0.85240600
H	1.20568500	-1.14436000	0.90541700

H	3.36913100	-0.23674900	0.00801100
H	2.48477900	1.01448500	-0.90938100
H	2.48341000	1.05194800	0.87108000
C	-1.20351200	-0.48028000	-0.01192700
C	-2.46000600	0.38509000	0.00546300
H	-1.20563800	-1.18170800	0.85240900
H	-1.20562100	-1.14430000	-0.90546800
H	-3.36915300	-0.23672200	-0.00837200
H	-2.48492200	1.01430600	0.90945300
H	-2.48321400	1.05211700	-0.87101000

³O₂

Charge = 0 Multiplicity = 3

O	0.00000000	0.00000000	0.59981400
O	0.00000000	0.00000000	-0.59981400

¹O₂

Charge = 0 Multiplicity = 1

O	0.00000000	0.00000000	0.60039600
O	0.00000000	0.00000000	-0.60039600

HO₂

Charge = 0 Multiplicity = 2

O	0.05544500	-0.60242800	0.00000000
O	0.05544500	0.71247200	0.00000000
H	-0.88711900	-0.88035600	0.00000000

TS-1

Charge = 0 Multiplicity = 2

C	1.69524700	-0.51308200	-0.79654500
C	-0.14255800	-0.10199700	1.23294700
C	0.78407900	-1.60773500	-0.48320800
N	-0.08475500	-1.33845700	0.58369200
N	0.73719500	0.85601600	0.76826900
N	1.55035400	0.72677600	-0.31805200
O	-0.91936000	0.10896100	2.15764900
O	0.78766600	-2.69701800	-1.04599600
C	0.62535500	2.22383000	1.29225200
H	0.31920500	2.15087200	2.34225700
H	1.63414000	2.65414800	1.24262300
C	-1.03690100	-2.37940200	1.00297500
H	-1.19333900	-2.25964500	2.08107700
H	-0.55077500	-3.34337000	0.81244000
C	-2.35201400	-2.29023200	0.25512400

C	-3.38683000	-1.46885400	0.73021600
C	-2.53610400	-2.99470900	-0.94490100
C	-4.58760900	-1.36092600	0.02207400
H	-3.23347700	-0.90348300	1.65173900
C	-3.73758200	-2.88798700	-1.65264900
H	-1.72180500	-3.61529700	-1.32607000
C	-4.76667000	-2.07136200	-1.17041100
H	-5.38675500	-0.71888900	0.40215300
H	-3.87054800	-3.44345500	-2.58485600
H	-5.70592300	-1.98764300	-1.72348500
C	-0.36033300	3.05462400	0.49824100
C	0.07075600	3.81111500	-0.60151900
C	-1.72871500	3.02677800	0.81320000
C	-0.84723300	4.53404000	-1.37028400
H	1.13305800	3.82857400	-0.85811700
C	-2.64722200	3.74825300	0.04498800
H	-2.06691400	2.42191800	1.65748100
C	-2.20849800	4.50424800	-1.04836400
H	-0.49887900	5.12226000	-2.22337000
H	-3.70990600	3.71977000	0.29991000
H	-2.92652800	5.06935100	-1.64839300
C	3.47204000	-1.39496900	0.31789100
H	3.67303800	-2.08330600	-0.50726000
C	2.94196000	-1.99244300	1.58608800
H	2.21227700	-2.78440300	1.37420500
H	3.76630500	-2.44534000	2.16722300
H	2.46467900	-1.23139900	2.22484300
N	4.31444900	-0.33739500	0.42946100
H	4.15371600	0.25748400	1.23857400
C	4.87588100	0.36506600	-0.72152800
C	5.52587900	-0.55991000	-1.74501900
H	5.62641400	1.06841600	-0.32935600
H	4.08834600	0.97501000	-1.20343700
H	6.01710000	0.04145500	-2.52473300
H	6.28533000	-1.20154300	-1.27077800
H	4.79143000	-1.20817800	-2.24752300
H	2.21508000	-0.59350100	-1.75336800

INT-1

Charge = 0 Multiplicity = 2

C	-1.42796800	-0.75818700	-0.10665300
C	0.86257200	0.14289700	-1.46687000
C	-1.39215700	0.66453000	-0.65492600
N	-0.19236200	1.03453200	-1.24323800

N	0.56792700	-1.20295100	-1.26599700
N	-0.56962000	-1.70453700	-0.77964500
O	1.95415900	0.51296000	-1.86549700
O	-2.30998800	1.45365400	-0.52881900
C	1.60500600	-2.19993600	-1.59861300
H	1.06052900	-3.08437000	-1.95331600
H	2.21279700	-1.79617100	-2.41581500
C	0.02003900	2.45624900	-1.59148200
H	-0.94910000	2.84456800	-1.92492200
H	0.72302500	2.47982400	-2.43116500
C	0.54735700	3.25847800	-0.42014300
C	-0.33877200	3.91459300	0.44878900
C	1.92717200	3.32610300	-0.16860200
C	0.14677900	4.63100500	1.54736700
H	-1.41343100	3.85035600	0.26367700
C	2.41228100	4.04237300	0.92957500
H	2.61525900	2.80189300	-0.83541500
C	1.52316600	4.69687200	1.78992600
H	-0.55232800	5.13971400	2.21626400
H	3.48860700	4.09047400	1.11455600
H	1.90268100	5.25771900	2.64802400
C	2.45780000	-2.52829200	-0.39314400
C	3.61758200	-1.78717500	-0.11771000
C	2.06558300	-3.54123000	0.49485000
C	4.37766400	-2.06209700	1.02309700
H	3.91097100	-0.98420600	-0.79777100
C	2.82473500	-3.81583100	1.63657100
H	1.15772800	-4.11455400	0.29007500
C	3.98316700	-3.07713300	1.90224800
H	5.28080300	-1.48115200	1.22730900
H	2.51222500	-4.60961200	2.31998000
H	4.57817100	-3.29229100	2.79357600
C	-2.85801700	-1.34526600	-0.00089000
H	-2.70093500	-2.38210700	0.34163600
C	-3.52955700	-1.39074500	-1.38553200
H	-2.85670200	-1.85508300	-2.12454200
H	-4.45819300	-1.97566600	-1.35966900
H	-3.77412400	-0.37356100	-1.72801100
N	-3.58189600	-0.65161800	1.05338700
H	-3.87433800	0.27124200	0.73880000
C	-4.63167900	-1.35169000	1.77631300
C	-5.95241100	-1.62121300	1.03862200
H	-4.85611500	-0.75828400	2.68091500
H	-4.21547400	-2.30766100	2.14204600

H	-6.70879100	-2.02135100	1.73447200
H	-6.35133600	-0.68960100	0.60310400
H	-5.83204200	-2.35083800	0.22352300
H	-1.06365700	-0.64600500	0.93889700

4a

Charge = 0 Multiplicity = 1

C	1.78789300	-0.06371100	-0.85261500
C	-0.84469500	0.07191300	-1.75426500
C	1.02523300	-1.32626800	-0.97199800
N	-0.27637000	-1.16447200	-1.44562500
N	0.01346400	1.15304900	-1.61906400
N	1.27494000	1.07951900	-1.15982200
O	-2.00337800	0.19203700	-2.11769200
O	1.47597200	-2.42581400	-0.68628700
C	-0.51454300	2.51514600	-1.81008200
H	0.30914100	3.11092400	-2.22286100
H	-1.31602100	2.44888100	-2.55490500
C	-1.14492600	-2.35610200	-1.54094900
H	-0.48852800	-3.20073200	-1.77874500
H	-1.83370700	-2.18527200	-2.37549500
C	-1.90338500	-2.60849100	-0.25395700
C	-1.32845800	-3.38118700	0.76782000
C	-3.17223500	-2.04272400	-0.05232200
C	-2.01357900	-3.58933100	1.96868600
H	-0.33397500	-3.80702100	0.61725500
C	-3.85708100	-2.25152800	1.14876900
H	-3.61244300	-1.42764400	-0.83990400
C	-3.27973900	-3.02536500	2.16168400
H	-1.55727300	-4.19404600	2.75675300
H	-4.84563300	-1.80819700	1.29458000
H	-3.81577900	-3.18869800	3.10026700
C	-1.02194100	3.10642900	-0.51229800
C	-2.29756200	2.76834900	-0.03069000
C	-0.20366700	3.94913500	0.25358900
C	-2.74589000	3.26966900	1.19434400
H	-2.92925000	2.09948200	-0.61963600
C	-0.65327300	4.45367700	1.47851900
H	0.79322400	4.21032100	-0.11154000
C	-1.92510800	4.11423600	1.95137600
H	-3.74033800	3.00098700	1.56006600
H	-0.00793200	5.11263200	2.06513400
H	-2.27711300	4.50748200	2.90858600
C	3.19854500	-0.11535100	-0.29317600
H	3.50785200	0.93728900	-0.19545000

C	4.16243100	-0.82723500	-1.25840900
H	4.15709000	-0.34514700	-2.24946700
H	5.18903500	-0.79867300	-0.86620300
H	3.86656600	-1.87918200	-1.38386700
N	3.12853700	-0.68578100	1.04941100
H	3.20626900	-1.69992300	1.01960000
C	3.94375800	-0.08708400	2.09438300
C	5.46710300	-0.16499800	1.92032300
H	3.66485100	-0.57195400	3.04591500
H	3.64484500	0.97186900	2.19834300
H	5.98163000	0.25699600	2.79969600
H	5.79604200	-1.21095000	1.80119000
H	5.80339800	0.39952800	1.03582300

H₂O₂

Charge = 0 Multiplicity = 1

O	-0.00000400	0.72582300	0.00000000
O	-0.00000400	-0.72580600	0.00000000
H	-0.95766200	0.88399400	0.00000000
H	0.95772000	-0.88413200	0.00000000

TS-2

Charge = 0 Multiplicity = 2

C	-1.62720800	-0.55241600	-0.61601300
C	0.85314000	0.10379300	-1.70076500
C	-1.36991800	0.85045100	-0.96304800
N	-0.09207500	1.11003300	-1.46599200
N	0.40647400	-1.18832100	-1.52886100
N	-0.82356800	-1.56995200	-1.08926800
O	1.99798200	0.36510500	-2.05523800
O	-2.16476900	1.76914800	-0.75368600
C	1.35377900	-2.29150000	-1.73539200
H	0.76244100	-3.13191200	-2.12246900
H	2.07590800	-1.97831500	-2.49822700
C	0.34338300	2.50965900	-1.60894800
H	-0.54179300	3.08763700	-1.89794200
H	1.07544300	2.54003700	-2.42357200
C	0.94196300	3.05602300	-0.32791600
C	0.12361400	3.67199400	0.63264000
C	2.31402700	2.91546100	-0.06494100
C	0.66850300	4.14671600	1.82994100
H	-0.94710600	3.76189600	0.43635300
C	2.85897700	3.38963100	1.13231000
H	2.94599500	2.41676900	-0.80275300

C	2.03796300	4.00763100	2.08249000
H	0.02173300	4.62740500	2.56888500
H	3.92926000	3.27640100	1.32463100
H	2.46443200	4.37949800	3.01789500
C	2.05732600	-2.66917500	-0.44904100
C	3.23021600	-2.00255400	-0.05928900
C	1.51103100	-3.64130700	0.40199000
C	3.84947200	-2.30977100	1.15580300
H	3.64217100	-1.22924900	-0.71167300
C	2.12942200	-3.94935300	1.61831100
H	0.59194500	-4.15520300	0.10868700
C	3.30089400	-3.28468300	1.99743700
H	4.76326500	-1.78567200	1.44820500
H	1.69607800	-4.71119000	2.27180100
H	3.78572900	-3.52588200	2.94704700
C	-3.08521000	-0.94171400	-0.34050200
H	-3.07843700	-2.02838200	-0.16720800
C	-4.13516300	-0.57327500	-1.37973900
H	-3.89373400	-1.07605500	-2.32894200
H	-5.14011300	-0.89568000	-1.07124200
H	-4.14628900	0.51140300	-1.55406400
N	-3.22581500	-0.29580700	1.01064200
H	-3.49156100	0.68630500	0.89577100
C	-3.96105900	-0.97018600	2.08769800
C	-5.45786500	-1.13921600	1.83377000
H	-3.79290400	-0.38099100	3.00270500
H	-3.48394000	-1.95066400	2.24732900
H	-5.94082100	-1.57864500	2.72056600
H	-5.93841100	-0.16900300	1.62824900
H	-5.65130500	-1.80811700	0.98158100
H	-1.85252600	-0.30534300	0.80335300

INT-1-pAcid

Charge = 0 Multiplicity = 2

C	-1.54108100	-1.17873300	-0.41737700
C	0.58159700	-0.97793500	-2.16891200
C	-1.60528600	-0.14861200	-1.45223800
N	-0.46277500	-0.04436500	-2.24170200
N	0.33086100	-2.10655100	-1.41305600
N	-0.75412600	-2.32130500	-0.62301900
O	1.63591000	-0.80595100	-2.76593900
O	-2.52018100	0.68203600	-1.55222000
C	1.41472700	-3.08615300	-1.24853200
H	0.92503000	-4.05634500	-1.09179300

H	1.98923600	-3.11952000	-2.18132300
C	-0.19625800	1.22532300	-2.94280100
H	-1.16796900	1.61644100	-3.26483100
H	0.41086800	0.99718500	-3.82530300
C	0.51105900	2.21231000	-2.03283600
C	-0.21577900	2.93456700	-1.07098500
C	1.90373200	2.37011200	-2.09011300
C	0.43686700	3.80009900	-0.18873700
H	-1.29718500	2.79836100	-1.00762100
C	2.55679200	3.24380700	-1.21385300
H	2.47606100	1.78821600	-2.81564800
C	1.82535300	3.96072700	-0.26119500
H	-0.13815200	4.34026100	0.56701300
H	3.64251600	3.35773500	-1.26972000
H	2.33587000	4.63271400	0.43322600
C	2.29982500	-2.72387100	-0.07397300
C	3.41257800	-1.88640600	-0.25214900
C	1.97062300	-3.15370500	1.21991300
C	4.19002600	-1.49885900	0.84265600
H	3.65008800	-1.52574500	-1.25505100
C	2.74555900	-2.76389000	2.31690200
H	1.09480600	-3.79079800	1.36681000
C	3.85935400	-1.93767400	2.13011400
H	5.05445900	-0.84690600	0.69217700
H	2.48017100	-3.10688400	3.32040600
H	4.46699900	-1.63365900	2.98640700
C	-2.84098800	-1.50142300	0.31422900
H	-2.58063600	-2.10898300	1.19441700
C	-3.84844200	-2.25240400	-0.55123400
H	-3.34758200	-3.14686400	-0.94742300
H	-4.73147600	-2.58097500	0.01605300
H	-4.17296900	-1.63302300	-1.40121100
N	-3.39948000	-0.20611700	0.84680700
H	-3.53456600	0.39643900	0.01133300
C	-4.62020300	-0.26884800	1.71274200
C	-5.90423700	0.03368300	0.95496600
H	-4.46738800	0.46650200	2.51554400
H	-4.64404500	-1.26285900	2.18228500
H	-6.75596000	-0.00527500	1.65004900
H	-5.87401800	1.04355400	0.51596700
H	-6.08986400	-0.68947200	0.14850100
H	-0.68822400	-0.48112900	0.45468400
C	0.84291100	1.89395100	2.50411700
O	0.51286000	2.83764900	3.18514300

C	2.26432600	1.50108400	2.21917900
H	2.43544300	1.51601200	1.13195100
H	2.95446500	2.18749800	2.72634700
H	2.43915200	0.46153200	2.53664100
C	-0.25697200	0.99795300	1.85945300
O	0.19864200	0.07045800	1.10094400
O	-1.44659700	1.22477200	2.10648000
H	-2.62803700	0.29201500	1.37560200

TS-2-pAcid

Charge = 0 Multiplicity = 2

C	-1.54108100	-1.17873300	-0.41737700
C	0.58159700	-0.97793500	-2.16891200
C	-1.60528600	-0.14861200	-1.45223800
N	-0.46277500	-0.04436500	-2.24170200
N	0.33086100	-2.10655100	-1.41305600
N	-0.75412600	-2.32130500	-0.62301900
O	1.63591000	-0.80595100	-2.76593900
O	-2.52018100	0.68203600	-1.55222000
C	1.41472700	-3.08615300	-1.24853200
H	0.92503000	-4.05634500	-1.09179300
H	1.98923600	-3.11952000	-2.18132300
C	-0.19625800	1.22532300	-2.94280100
H	-1.16796900	1.61644100	-3.26483100
H	0.41086800	0.99718500	-3.82530300
C	0.51105900	2.21231000	-2.03283600
C	-0.21577900	2.93456700	-1.07098500
C	1.90373200	2.37011200	-2.09011300
C	0.43686700	3.80009900	-0.18873700
H	-1.29718500	2.79836100	-1.00762100
C	2.55679200	3.24380700	-1.21385300
H	2.47606100	1.78821600	-2.81564800
C	1.82535300	3.96072700	-0.26119500
H	-0.13815200	4.34026100	0.56701300
H	3.64251600	3.35773500	-1.26972000
H	2.33587000	4.63271400	0.43322600
C	2.29982500	-2.72387100	-0.07397300
C	3.41257800	-1.88640600	-0.25214900
C	1.97062300	-3.15370500	1.21991300
C	4.19002600	-1.49885900	0.84265600
H	3.65008800	-1.52574500	-1.25505100
C	2.74555900	-2.76389000	2.31690200
H	1.09480600	-3.79079800	1.36681000
C	3.85935400	-1.93767400	2.13011400

H	5.05445900	-0.84690600	0.69217700
H	2.48017100	-3.10688400	3.32040600
H	4.46699900	-1.63365900	2.98640700
C	-2.84098800	-1.50142300	0.31422900
H	-2.58063600	-2.10898300	1.19441700
C	-3.84844200	-2.25240400	-0.55123400
H	-3.34758200	-3.14686400	-0.94742300
H	-4.73147600	-2.58097500	0.01605300
H	-4.17296900	-1.63302300	-1.40121100
N	-3.39948000	-0.20611700	0.84680700
H	-3.53456600	0.39643900	0.01133300
C	-4.62020300	-0.26884800	1.71274200
C	-5.90423700	0.03368300	0.95496600
H	-4.46738800	0.46650200	2.51554400
H	-4.64404500	-1.26285900	2.18228500
H	-6.75596000	-0.00527500	1.65004900
H	-5.87401800	1.04355400	0.51596700
H	-6.08986400	-0.68947200	0.14850100
H	-0.68822400	-0.48112900	0.45468400
C	0.84291100	1.89395100	2.50411700
O	0.51286000	2.83764900	3.18514300
C	2.26432600	1.50108400	2.21917900
H	2.43544300	1.51601200	1.13195100
H	2.95446500	2.18749800	2.72634700
H	2.43915200	0.46153200	2.53664100
C	-0.25697200	0.99795300	1.85945300
O	0.19864200	0.07045800	1.10094400
O	-1.44659700	1.22477200	2.10648000
H	-2.62803700	0.29201500	1.37560200

INT-2-pAcid

Charge = 0 Multiplicity = 2

C	1.73155900	-1.37141600	0.21402900
C	-0.27240000	-1.24923200	2.12660500
C	1.97758800	-0.60833400	1.37292600
N	0.88610400	-0.48721700	2.26795900
N	-0.34791300	-2.01640600	0.98782300
N	0.53270000	-1.93945700	-0.08327300
O	-1.16958300	-1.22217800	2.96566300
O	3.04893300	0.02210800	1.60508100
C	-1.50735300	-2.88402800	0.77979400
H	-1.14346100	-3.78250100	0.26230200
H	-1.86735800	-3.17441100	1.77546300
C	0.79626600	0.71629400	3.10909100

H	1.82273500	1.00657000	3.35966800
H	0.25646100	0.45663500	4.02668000
C	0.08220200	1.80822900	2.33460400
C	0.76448600	2.50968200	1.32590500
C	-1.29069000	2.03802500	2.51176100
C	0.08728400	3.41845000	0.50877200
H	1.82809700	2.31360700	1.17151000
C	-1.96916400	2.95239800	1.69850800
H	-1.83062600	1.47673200	3.27758700
C	-1.28274700	3.64137100	0.69248800
H	0.62128300	3.93552200	-0.29152000
H	-3.03977000	3.11910000	1.84384300
H	-1.81377900	4.34353800	0.04485700
C	-2.63319800	-2.24024700	-0.00733000
C	-3.37773900	-1.18784500	0.55354600
C	-2.94782700	-2.67938400	-1.29924800
C	-4.41773800	-0.59513700	-0.16511200
H	-3.12750600	-0.84138600	1.55823700
C	-3.99145900	-2.08735200	-2.02093800
H	-2.36964800	-3.49259700	-1.74733600
C	-4.72983200	-1.04457400	-1.45469900
H	-4.98939400	0.22249500	0.28209100
H	-4.22584200	-2.44172200	-3.02824200
H	-5.54449300	-0.57996700	-2.01627400
C	2.82045800	-1.50558700	-0.82161500
H	2.36235400	-1.81211100	-1.77422000
C	3.89523900	-2.51268900	-0.41457000
H	3.40879500	-3.48342600	-0.24409900
H	4.65926500	-2.65165200	-1.19443400
H	4.38078800	-2.19906700	0.52102800
N	3.38706700	-0.12047400	-1.04395500
H	3.60197400	0.21906700	-0.07209000
C	4.52736100	0.05536500	-1.99530700
C	5.87954600	0.10287800	-1.29906200
H	4.34195100	0.99694100	-2.53142100
H	4.47381300	-0.75506000	-2.73670500
H	6.67009500	0.26347700	-2.04696300
H	5.92169300	0.93529600	-0.57902000
H	6.10391400	-0.82908300	-0.76192900
H	-0.17277100	-0.94542500	-1.15781400
C	-1.09923600	2.03887800	-2.33804600
O	-0.62081900	3.04969500	-2.79619200
C	-2.56512900	1.80171800	-2.13063900
H	-2.75345900	1.60569500	-1.06324700

H	-3.13779400	2.67436400	-2.46913200
H	-2.88524500	0.89085100	-2.65889600
C	-0.13202000	0.89898500	-1.90125700
O	-0.75545100	-0.20105100	-1.58595500
O	1.07205500	1.09324500	-1.88481000
H	2.56840500	0.44016500	-1.36130700

TS-3-pAcid

Charge = 0 Multiplicity = 2

C	1.70724300	-1.53742800	-1.03852900
C	-0.36940300	-0.05686100	-2.21901800
C	0.40455100	-2.18014600	-1.19327000
N	-0.59266700	-1.35722900	-1.75616500
N	0.90320300	0.42310200	-2.01504900
N	1.86300000	-0.18963400	-1.25468400
O	-1.24765800	0.59549200	-2.77046700
O	0.13378300	-3.33101800	-0.86119500
C	1.24253600	1.77875000	-2.46569300
H	2.29304500	1.74115600	-2.78370100
H	0.61430700	1.99269200	-3.33847800
C	-1.95037400	-1.89634300	-1.91619500
H	-1.84580800	-2.98737800	-1.94570000
H	-2.33992400	-1.54561800	-2.87872500
C	-2.88103000	-1.49298600	-0.79046600
C	-2.67855700	-1.99642500	0.50591400
C	-3.95275600	-0.61920800	-1.02069700
C	-3.54068100	-1.64107800	1.54658100
H	-1.83697000	-2.66740900	0.69166100
C	-4.82141900	-0.26929200	0.01975600
H	-4.10243200	-0.20682800	-2.02146800
C	-4.61824300	-0.78056700	1.30519700
H	-3.36208800	-2.02618500	2.55290100
H	-5.65395200	0.41211400	-0.17361000
H	-5.28965200	-0.50082900	2.12079100
C	1.04391300	2.83110300	-1.39617300
C	-0.21073500	3.43350400	-1.21958800
C	2.09430300	3.17677700	-0.53370000
C	-0.40882000	4.37175500	-0.20305300
H	-1.03470100	3.14462400	-1.87626100
C	1.89513400	4.10715500	0.49139200
H	3.07321300	2.70774200	-0.66403000
C	0.64280700	4.70778200	0.65805200
H	-1.38899600	4.83926400	-0.07794400
H	2.72050100	4.36681600	1.15951800

H	0.48665300	5.43897000	1.45547200
C	2.83722900	-2.22098100	-0.52352400
H	3.76052500	-1.65986100	-0.68499600
C	2.98694200	-3.71600900	-0.49790800
H	2.94853600	-4.10862900	-1.52805200
H	3.95623500	-3.99725400	-0.06132700
H	2.17295400	-4.19874200	0.05538300
N	2.92166000	-1.86645800	1.50426800
H	3.30917500	-2.67388500	1.99625400
C	3.62559400	-0.62464900	1.84282800
C	5.13757700	-0.78525700	1.75704200
H	3.33723000	-0.28400700	2.85421000
H	3.28465800	0.14942300	1.13583900
H	5.63793800	0.16409000	1.99995300
H	5.49529000	-1.54714700	2.46957600
H	5.45622800	-1.08791300	0.74718100
H	1.06126300	0.46054400	0.36180300
C	-1.46354100	0.67037700	2.45653700
O	-1.75331400	0.28023100	3.56252600
C	-2.21025200	1.71042300	1.67801300
H	-2.51895200	1.29008000	0.70690200
H	-3.08959200	2.04129100	2.24379100
H	-1.54273300	2.55648800	1.45230300
C	-0.21942000	0.04693600	1.76879500
O	0.29054300	0.85031900	0.85296300
O	0.20839700	-1.04416200	2.07641500
H	1.92207800	-1.79296200	1.72646000

INT-2

Charge = 0 Multiplicity = 2

C	-1.46791600	-1.06208200	-0.48876400
C	0.69253900	0.03505800	-1.81400400
C	-1.55558400	0.28478700	-0.87069600
N	-0.42854400	0.81474200	-1.54947100
N	0.60530300	-1.29232500	-1.45083900
N	-0.42893200	-1.88491900	-0.75244700
O	1.69851200	0.51008500	-2.34028900
O	-2.54857700	1.05435600	-0.61681200
C	1.79273700	-2.13662600	-1.57717900
H	1.44093500	-3.14658000	-1.83047900
H	2.39044800	-1.74804300	-2.41042100
C	-0.30760200	2.26636700	-1.71697600
H	-1.32486800	2.65435500	-1.84440800
H	0.26758800	2.45162500	-2.63169300

C	0.36454300	2.91611200	-0.52141000
C	-0.37304200	3.18124200	0.64479800
C	1.73896700	3.19880300	-0.53489300
C	0.25038500	3.72710100	1.77077300
H	-1.43831800	2.93794700	0.65675500
C	2.36347400	3.74619700	0.59106800
H	2.31893800	2.96822000	-1.43112600
C	1.62100100	4.01226000	1.74686200
H	-0.33479400	3.93208700	2.67159000
H	3.43489300	3.96306300	0.56689500
H	2.10891700	4.43934600	2.62709900
C	2.60885000	-2.15980000	-0.29963500
C	3.39243700	-1.04776400	0.05494500
C	2.55008800	-3.25391200	0.57432000
C	4.10451000	-1.03592800	1.25701800
H	3.42495500	-0.18798600	-0.61828900
C	3.26536900	-3.24539200	1.77771800
H	1.93469900	-4.11875000	0.31147800
C	4.04415200	-2.13605800	2.12198900
H	4.70996500	-0.16462800	1.52109300
H	3.21146500	-4.10672300	2.44907100
H	4.60274600	-2.12737600	3.06172400
C	-2.67066600	-1.69700200	0.17021000
H	-2.34195200	-2.57750200	0.74205100
C	-3.74115600	-2.10523100	-0.84103400
H	-3.27682400	-2.80894900	-1.54609300
H	-4.60112700	-2.61135300	-0.37662100
H	-4.09185600	-1.23055700	-1.40828500
N	-3.19326500	-0.68204500	1.17032900
H	-3.18641100	0.22783400	0.57807300
C	-4.48501500	-0.94770600	1.88046400
C	-5.67764000	-0.28557600	1.20562000
H	-4.36650600	-0.55629100	2.90032800
H	-4.60789700	-2.03764800	1.96367600
H	-6.58237200	-0.47751700	1.80133600
H	-5.53774700	0.80484200	1.14266500
H	-5.85144600	-0.67007900	0.19169500
H	-2.44743600	-0.54214400	1.85852800

TS-3

Charge = 0 Multiplicity = 2

C	0.92040100	-1.32067200	-1.40873200
C	-1.00357400	0.64544200	-1.91949200
C	-0.46835600	-1.66862600	-1.21348500

N	-1.38656200	-0.65333200	-1.58467700
N	0.35063200	0.83974700	-2.07970000
N	1.32310100	-0.09577200	-1.86771000
O	-1.82361500	1.55009300	-2.06101000
O	-0.89817800	-2.74139700	-0.78152400
C	0.87322600	2.21175800	-2.06809300
H	1.71614400	2.25138400	-2.77211900
H	0.07765400	2.87822000	-2.41867900
C	-2.81871600	-0.89861000	-1.35816800
H	-2.99618000	-1.95919200	-1.56970500
H	-3.37190200	-0.28832300	-2.08130400
C	-3.24941500	-0.56346700	0.05902300
C	-3.20051000	-1.53841600	1.06868000
C	-3.66693100	0.73603600	0.39081100
C	-3.56460000	-1.22202300	2.38151400
H	-2.85474900	-2.54248100	0.81547800
C	-4.02938800	1.05331100	1.70380300
H	-3.68787700	1.49889700	-0.38949800
C	-3.97959500	0.07509700	2.70342900
H	-3.52418500	-1.99191500	3.15697400
H	-4.35355800	2.06880800	1.94727900
H	-4.26463200	0.32245300	3.72953800
C	1.31685200	2.55920000	-0.66090000
C	0.35954400	2.88727200	0.31287000
C	2.65774300	2.41601500	-0.27407000
C	0.73607100	3.06815000	1.64708600
H	-0.68943000	2.97689500	0.01888500
C	3.03697200	2.59444200	1.06203500
H	3.40658100	2.15021500	-1.02447700
C	2.07579300	2.91893700	2.02594100
H	-0.01981600	3.32063600	2.39526800
H	4.08527200	2.47943600	1.35059400
H	2.36992800	3.05653700	3.06962000
C	1.99825700	-2.11750100	-0.90347400
H	2.94853800	-1.88742200	-1.39966200
C	1.85677300	-3.55249000	-0.48025000
H	1.52705100	-4.15170000	-1.34374400
H	2.82054600	-3.95243000	-0.13462800
H	1.09437800	-3.67770700	0.29820300
N	2.51606200	-1.15364900	0.67219200
H	1.72248000	-1.21123000	1.31574900
C	3.80371900	-1.42851200	1.33579200
C	3.67686800	-2.47106000	2.43814000
H	4.20848600	-0.48852300	1.74837500

H	4.50915400	-1.76314200	0.55623300
H	4.66208100	-2.66748200	2.88647100
H	3.00636600	-2.11730400	3.23848200
H	3.28092500	-3.42281100	2.05498700
H	2.49165000	-0.21605100	0.25648100

INT-3

Charge = 0 Multiplicity = 2

C	0.21281900	2.57625400	0.19317800
C	-0.10223500	0.37054000	-1.51422400
C	1.42108100	1.79983300	-0.20742700
N	1.16981000	0.73561400	-1.07227900
N	-1.13367600	1.18894600	-1.07540200
N	-1.01144000	2.23125300	-0.24672500
O	-0.29773000	-0.59428500	-2.23551800
O	2.55133900	2.04815100	0.17692600
C	-2.51820500	0.80703200	-1.41171600
H	-3.08773000	1.74409100	-1.44061400
H	-2.50502200	0.36265100	-2.41338400
C	2.30354600	-0.12066400	-1.47822200
H	3.18198100	0.53091200	-1.54369400
H	2.06775200	-0.50989500	-2.47464700
C	2.54386100	-1.25186400	-0.49898000
C	3.43338200	-1.08647600	0.57421800
C	1.85316900	-2.46713600	-0.63359700
C	3.63502900	-2.12129700	1.49291900
H	3.95668700	-0.13489300	0.69006900
C	2.05403900	-3.50097500	0.28593700
H	1.14880800	-2.59003500	-1.45913700
C	2.94633200	-3.33104400	1.35062400
H	4.33211400	-1.98231700	2.32345000
H	1.51252100	-4.44353700	0.17038200
H	3.10460300	-4.14017800	2.06839900
C	-3.09277900	-0.15580600	-0.39515200
C	-2.97477800	-1.54234000	-0.57897700
C	-3.69943700	0.33015700	0.77322500
C	-3.46256400	-2.42779600	0.38702600
H	-2.48555800	-1.92141700	-1.47883900
C	-4.18648400	-0.55479400	1.73992300
H	-3.78573400	1.40913500	0.92573400
C	-4.06934900	-1.93614700	1.54819700
H	-3.36791500	-3.50584600	0.23305500
H	-4.66035500	-0.16541300	2.64471500
H	-4.45131700	-2.62860100	2.30280100

C	0.30639200	3.68067100	1.04252200
H	-0.65491800	4.15583000	1.26104400
C	1.53945700	4.25144500	1.65837300
H	2.28007900	4.53882300	0.89312100
H	1.29678900	5.13213000	2.26904300
H	2.05583100	3.50938600	2.29099700

NH₂Et

Charge = 0 Multiplicity = 1

C	-0.05220300	0.55567600	0.05273200
C	1.24962300	-0.23615900	-0.02657600
H	-0.06934900	1.30898100	-0.75490100
H	-0.06620300	1.12992100	1.00511700
H	2.12603800	0.42557100	0.06263100
H	1.30826400	-0.97995500	0.78699800
H	1.31539500	-0.77990200	-0.98284200
N	-1.20956100	-0.32409800	-0.12346100
H	-1.26089500	-0.97549500	0.66311700
H	-2.07083900	0.22246500	-0.07282800

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